INVENTOR SEARCH

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=> fil capl; d que l113; d que l116; s l113,l116
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FILE COVERS 1907 - 2 Feb 2007  VOL 146 ISS 7
FILE LAST UPDATED: 1 Feb 2007  (20070201/ED)

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'OBI' IS DEFAULT SEARCH FIELD FOR 'CAPLUS' FILE


L106      14460 SEA FILE=CAPLUS ABB=ON  KIM M?/AU
L107      25330 SEA FILE=CAPLUS ABB=ON  PARK J?/AU
L108       4144 SEA FILE=CAPLUS ABB=ON  CHUNG Y?/AU
L109      11169 SEA FILE=CAPLUS ABB=ON  CHOI J?/AU
L110      29440 SEA FILE=CAPLUS ABB=ON  LEE H?/AU
L111       8289 SEA FILE=CAPLUS ABB=ON  CHOI Y?/AU
L112      23463 SEA FILE=CAPLUS ABB=ON  KIM D?/AU
L113          1 SEA FILE=CAPLUS ABB=ON  L106 AND L107 AND L108 AND L109 AND
                L110 AND L111 AND L112



L17      150091 SEA FILE=CAPLUS ABB=ON  ALCOHOLS/CT
L19       18354 SEA FILE=CAPLUS ABB=ON  L17(L)PREP/RL
L20         136 SEA FILE=CAPLUS ABB=ON  L19(L)"S"/OBI
L22       23387 SEA FILE=CAPLUS ABB=ON  "RESOLUTION (SEPARATION)"+OLD/CT
L28         995 SEA FILE=CAPLUS ABB=ON  DYNAMIC/OBI(L)KINETIC/OBI
L29         226 SEA FILE=CAPLUS ABB=ON  L28(L)L22
L35        3653 SEA FILE=CAPLUS ABB=ON  CHIRAL/OBI(L)(ALCOHOL/OBI OR ALCS/OBI)

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L107      25330 SEA FILE=CAPLUS ABB=ON  PARK J?/AU
L108       4144 SEA FILE=CAPLUS ABB=ON  CHUNG Y?/AU
L109      11169 SEA FILE=CAPLUS ABB=ON  CHOI J?/AU
L110      29440 SEA FILE=CAPLUS ABB=ON  LEE H?/AU
L111       8289 SEA FILE=CAPLUS ABB=ON  CHOI Y?/AU
L112      23463 SEA FILE=CAPLUS ABB=ON  KIM D?/AU
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                OR (L111 AND L112)
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L117          17 (L113 OR L116)

=> fil casrea; d que nos 197
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FILE CONTENT:1840 - 28 Jan 2007 VOL 146 ISS 5

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*                                                          *
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database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance
identification.


L14      152839 SEA FILE=REGISTRY ABB=ON  RU/ELS
L24           1 SEA FILE=REGISTRY ABB=ON  SUBTILISIN/CN
L25           1 SEA FILE=REGISTRY ABB=ON  PROTEINASE/CN
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L60         448 SEA FILE=CASREACT ABB=ON  PARK J?/AU
L61         212 SEA FILE=CASREACT ABB=ON  CHUNG Y?/AU
L62         255 SEA FILE=CASREACT ABB=ON  CHOI J?/AU
L63         702 SEA FILE=CASREACT ABB=ON  LEE H?/AU
L64         126 SEA FILE=CASREACT ABB=ON  CHOI Y?/AU
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PROCESSING COMPLETED FOR L97
PROCESSING COMPLETED FOR L117
L118         24 DUP REM L97 L117 (6 DUPLICATES REMOVED)
                ANSWERS '1-13' FROM FILE CASREACT
                ANSWERS '14-24' FROM FILE CAPLUS

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'ED' IS NOT A VALID FORMAT
REENTER DISPLAY FORMAT FOR ALL FILES (FILEDEFAULT):end

=> d ibib abs fhit 1-13; d ibib ed abs hitind 14-24


L118 ANSWER 1 OF 24  CASREACT  COPYRIGHT 2007 ACS on STN DUPLICATE 1
ACCESSION NUMBER:         142:197677  CASREACT  Full-text
TITLE:                    Method of preparation of optically active alcohols
INVENTOR(S):              Kim, Mahn-Joo; Park, JaiWook;
                          Chung, Yong Il; Choi, Jun Ho;
                          Lee, Han Ki; Choi, Yoon Kyung;
                          Kim, Daeho
PATENT ASSIGNEE(S):       Postech Foundation, S. Korea; Posco
SOURCE:                   PCT Int. Appl., 34 pp.
                          CODEN: PIXXD2
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

     PATENT NO.        KIND  DATE          APPLICATION NO.  DATE
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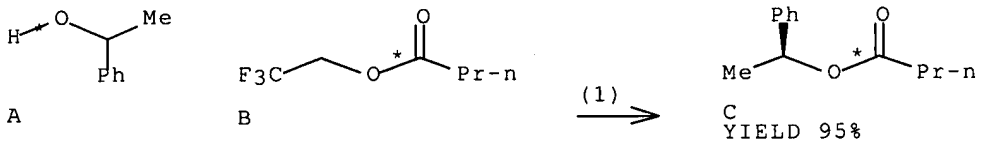
     WO 2005009935      A1   20050203      WO 2003-KR1494   20030725
         W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM,
             PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN,
             TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
             KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,
             FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR,
             BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
     AU 2003247201      A1   20050214      AU 2003-247201   20030725
     US 2007015943      A1   20070118      US 2006-565829   20060825
PRIORITY APPLN. INFO.:                    WO 2003-KR1494   20030725
OTHER SOURCE(S):          MARPAT 142:197677
AB   The present invention relates to a method for preparing chiral alc. having
     optical activity.  More specifically, the present invention relates to a
```

method for preparing (S)-chiral alc. with a high yield and a high optical purity by mixing achiral substrates such as racemic alc. or ketone with a combination of metal catalyst and protein hydrolase to perform a dynamic kinetic resolution reaction. Thus, to a Schlenk flask, 3.7 mg (Ph4C5NHCHMe2)Ru(CO)2Cl and 18 μl t-BuOK solution (1 M in THF) was added and dried under the reduced pressure, followed by adding 1 mL toluene and then the resulting mixture was agitated for 1 h. After the toluene was removed under the reduced pressure, 9 mg stabilized subtilisin, 31.8 mg Na2CO3, 18 μL 1-phenylethanol, 39 μL 2,2,2-trifluoroethyl butyrate, and 0.5 mL THF were added and the mixture was agitated at room temperature for 3 days. After termination of the reaction, catalyst was filtered, the obtained filtered solution was concentrated and separated using column chromatog. (silica gel, Et acetate/ hexane = 4:1) to give (S)-1-phenylethyl butyrate (I) % yield and optical purity 92% ee. (S)-(-)-phenylethanol was obtained by adding I and 2 equiv of K2CO3 to 80% methanol solution and hydrolyzing at room temperature

RX(1) OF 29 **A** + B ===> C...



RX(1)

STAGE(1)
RGT D 865-47-4 t-BuOK
CAT **470688-18-7** Ruthenium, dicarbonylchloro[(1,2,3,4,5-η)-1-[(1-methylethyl)amino]-2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl]-
SOL 109-99-9 THF, 108-88-3 PhMe
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) 1 hour, room temperature

STAGE(2)
RCT A **98-85-1**, B 371-27-7
RGT E 497-19-8 Na2CO3
CAT **9014-01-1** Subtilisin
SOL 109-99-9 THF
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) 72 hours, room temperature

PRO C **161024-76-6**
NTE **stereoselective**

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L118 ANSWER 2 OF 24 CASREACT COPYRIGHT 2007 ACS on STN DUPLICATE 2
ACCESSION NUMBER: 140:321067 CASREACT Full-text
TITLE: Aminocyclopentadienyl ruthenium complexes as racemization catalysts for dynamic kinetic resolution

of secondary alcohols at ambient temperature

AUTHOR(S): **Choi, Jun Ho; Choi, Yoon Kyung;** Kim, Yu Hwan; Park, Eun Sil; Kim, Eun Jung; **Kim, Mahn-Joo; Park, Jaiwook**

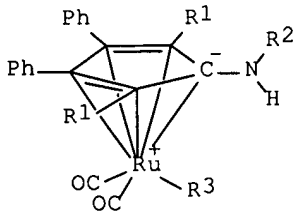
CORPORATE SOURCE: National Research Laboratory of Chirotechnology, Department of Chemistry, Division of Molecular and Life Sciences, Pohang University of Science and Technology, Pohang, 790-784, S. Korea

SOURCE: Journal of Organic Chemistry (2004), 69(6), 1972-1977
CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

got it.

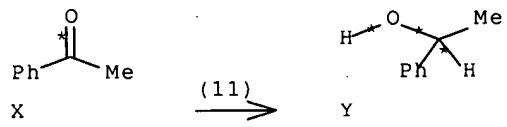
GI



I

AB Aminocyclopentadienyl ruthenium complexes I [R1 = Ph; R2 = i-Pr (II), n-Pr, t-Bu, Ph, 4-O2NC6H4, 4-ClC6H4, 4-MeOC6H4, 4-Me2NC6H4; R3 = Cl; R1 = Me; R2 = i-Pr (III), Ph; R3 = Cl] which can be used as room-temperature racemization catalysts with lipase in the dynamic kinetic resolution (DKR) of secondary alcs., were synthesized from iminocyclopenta-2,4-dienes, Ru3(CO)12, and CHCl3. The racemization of (S)-4-phenyl-2-butanol showed that III was the most active catalyst, although the difference decreased in the DKR. II was used in the DKR of various alcs. such as allylic alcs., alkynyl alcs., diols, hydroxy esters, and chlorohydrins, which were successfully transformed to chiral acetates. Mechanistic studies for the catalytic racemization, indicated that ruthenium hydride I [R1 = Ph; R2 = i-Pr; R3 = H (IV)] was the key species in the reaction. IV was the major organometallic species in the racemization of (S)-1-phenylethanol with II and potassium tert-butoxide. In a sep. experiment, (S)-1-phenylethanol was racemized catalytically by IV in the presence of acetophenone.

RX(11) OF 59 **X** ===> **Y**...



RX(11) RCT X **98-86-2**

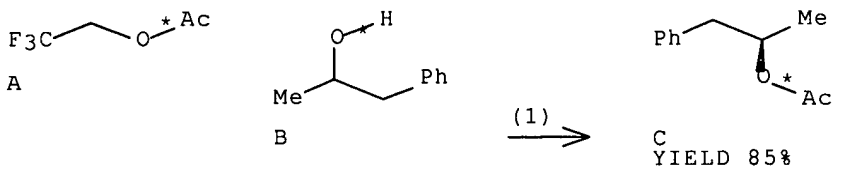
PRO Y 98-85-1
CAT 600136-37-6 Ruthenium, dicarbonylhydro[(1,2,3,4,5-η)-1-[(1-methylethyl)amino]-2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl]-, 67-63-0 Me2CHOH
SOL 67-63-0 Me2CHOH, 108-88-3 PhMe
CON 20 hours, 70 deg C
REFERENCE COUNT: 109 THERE ARE 109 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L118 ANSWER 3 OF 24 CASREACT COPYRIGHT 2007 ACS on STN DUPLICATE 3
ACCESSION NUMBER: 143:133122 CASREACT Full-text
TITLE: Dynamic kinetic resolution of secondary alcohols by enzyme-metal combinations in ionic liquid
AUTHOR(S): **Kim, Mahn-Joo**; Kim, Hyun Min; **Kim, Daeho**; Ahn, Yangsoo; **Park, Jaiwook**
CORPORATE SOURCE: National Research Laboratory of Chirotechnology, Department of Chemistry, Division of Molecular and Life Sciences, Pohang University of Science and Technology, Pohang, 790-784, S. Korea
SOURCE: Green Chemistry (2004), 6(9), 471-474
CODEN: GRCHFJ; ISSN: 1463-9262
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English

→ got it.

AB Secondary aralkyl alcs. undergo enantioselective acylation in ionic liqs. in the presence of bis(cymenedichlororuthenium) and either lipase or subtilisin. In ionic liqs. such as [BMIM+]PF6 (BMIM+ = 1-butyl-3-methylimidazolium), bis(cymenedichlororuthenium) racemizes secondary alcs. such as (S)-1-phenylethanol efficiently; the ruthenium complex racemizes secondary alcs. less effectively in conventional solvents such as methylene chloride, toluene, or THF. Secondary alcs. undergo enantioselective acylation and dynamic kinetic resolution with 2,2,2-trifluoroethyl acetate in the presence of bis(cymenedichlororuthenium) and lipase in [BMIM+]PF6- to give the (R)-secondary acetates in 85-92% yields and in 99% ee. In the presence of bis(cymenedichlororuthenium) and subtilisin in [BMIM+]PF6-, secondary alcs. undergo acylation with 2,2,2-trifluoroethyl butyrate to give the secondary butyrate esters in 78-92% yields and in 85-99% ee; dialcs. are acylated to diesters in 52-63% diastereoselectivities.

RX(1) OF 25 A + B ===> C



RX(1) RCT A 406-95-1, B 698-87-3
RGT D 121-44-8 Et3N
PRO C 116907-36-9

CAT 52462-29-0 Ruthenium, di-μ-chlorodichlorobis[(1,2,3,4,5,6-η)-1-methyl-4-(1-methylethyl)benzene]di-, 9001-62-1 Lipase
SOL 174501-64-5 1H-Imidazolium, 1-butyl-3-methyl-, hexafluorophosphate(1-)
CON 2 days, room temperature
NTE **stereoselective**, enantioselective, biotransformation, enzymic, 99% ee

REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L118 ANSWER 4 OF 24 CASREACT COPYRIGHT 2007 ACS on STN DUPLICATE 4
ACCESSION NUMBER: 139:261424 CASREACT Full-text
TITLE: Resolution of chiral compounds using aminocyclopentadienyl ruthenium catalysts
INVENTOR(S): **Park, Jaiwook; Kim, Mahn-joo; Choi, Jun Ho**; Ahn, Yangsoo
PATENT ASSIGNEE(S): Postech Foundation, S. Korea
SOURCE: PCT Int. Appl., 21 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

→ got it.

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003076384	A1	20030918	WO 2002-KR926	20020517
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
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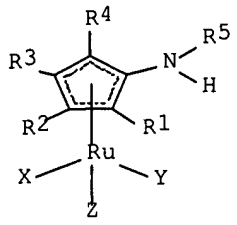
KR 2003074851	A	20030922	KR 2002-13832	20020314
CA 2478408	A1	20030918	CA 2002-2478408	20020517
AU 2002258278	A1	20030922	AU 2002-258278	20020517
EP 1483229	A1	20041208	EP 2002-728244	20020517
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
CN 1622932	A	20050601	CN 2002-828550	20020517
US 2005130282	A1	20050616	US 2004-507727	20040913
US 7156731	B2	20070102		
PRIORITY APPLN. INFO.:			KR 2002-13832	20020314
			WO 2002-KR926	20020517

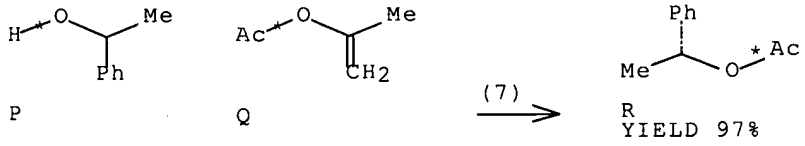
OTHER SOURCE(S): MARPAT 139:261424
GI



I

AB A chiral compound, particularly a chiral secondary alc., can be efficiently resolved under a mild condition by acylation with an alkenyl acetate in the presence of a novel aminocyclopentadienyl ruthenium complexes, I (preparation given; R1-R4 = (un)substituted Ph, C1-5 alkyl, etc.; R5 = H, (un)substituted Ph, C1-5 alkyl, C3-7 cycloalkyl, C2-5 alkenyl, C2-5 alkynyl, etc.; X, Y, Z = H, halo, CO, organophosphine), an enzyme catalyst, and a base. Thus, TiCl4-mediated reaction of tetraphenylcyclopentadienone with isobutylamine in PhMe gave N-isobutyl-2,3,4,5-tetraphenylcyclopentadieneimine which on treatment with Ru3(CO)12 gave title catalyst, N-isobutylamino-2,3,4,5-tetraphenylcyclopentadienylruthenium dicarbonyl chloride (II). . II catalyzed resolution of 1-phenylethanol in presence of Na2CO3/KOBu-t/Candida antarctica lipase B and isopropenyl acetate gave 97% (R)-1-phenylethyl acetate with 99% enantiomeric excess.

RX(7) OF 15 **P** + Q ===> **R**



P Q R
YIELD 97%

RX(7) RCT P **98-85-1**, Q 108-22-5
RGT S 865-47-4 t-BuOK, M 497-19-8 Na2CO3
PRO R **16197-92-5**
CAT **600136-35-4** Ruthenium, dicarbonylchloro[(1,2,3,4,5-η)-1-[(2-methylpropyl)amino]-2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl]-
SOL 108-88-3 PhMe
CON 30 hours, room temperature
NTE enzymic, **stereoselective**, Candida antatctica lipase B, biotransformation

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L118 ANSWER 5 OF 24 CASREACT COPYRIGHT 2007 ACS on STN DUPLICATE 5
ACCESSION NUMBER: 139:337584 CASREACT Full-text
TITLE: (S)-Selective Dynamic Kinetic Resolution of Secondary Alcohols by the Combination of Subtilisin and an

Aminocyclopentadienylruthenium Complex as the Catalysts

AUTHOR(S): **Kim, Mahn-Joo; Chung, Yong Il; Choi, Yoon Kyung; Lee, Han Ki; Kim, Daeho; Park, Jaiwook**

CORPORATE SOURCE: National Research Laboratory of Chirotechnology, Department of Chemistry, Division of Molecular and Life Sciences, Pohang University of Science and Technology, Kyongbuk, 790-784, S. Korea

SOURCE: Journal of the American Chemical Society (2003), 125(38), 11494-11495
CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society

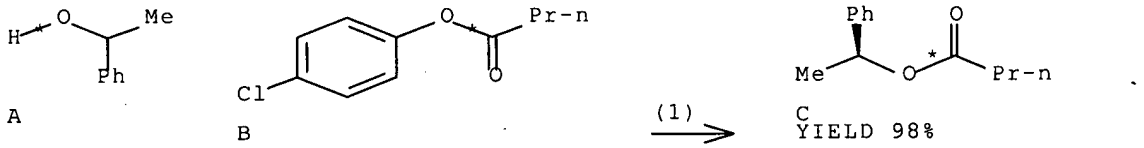
DOCUMENT TYPE: Journal

LANGUAGE: English

→ go + 4.

AB A new procedure for the dynamic kinetic resolution (DKR) of racemic alcs. into single enantiomers is described. This procedure employs surfactant-treated subtilisin as an (S)-selective resolving catalyst and an aminocyclopentadienylruthenium complex as a racemizing catalyst. The DKR is performed best in the presence of an acyl donor such as trifluoroethyl butyrate in THF at room temperature Eight simple secondary alcs. have been efficiently resolved with high optical purities and good yields. The subtilisin-based DKR is complementary in stereoselectivity to its lipase-based counterpart. For an acyl-carrying alc., both subtilisin- and lipase-based DKRs have proceeded equally well to give a pair of enantiomeric products (>99.5% ee each) with opposite optical rotations in high yields (94-95%).

RX(1) OF 13 **A** + B ===> C



RX(1)

STAGE(1)
RGT D 9004-95-9 Poly(oxy-1,2-ethanediyl), α-hexadecyl-ω-hydroxy-
CAT **9014-01-1** Subtilisin
SOL 110-86-1 Pyridine, 7732-18-5 Water
CON SUBSTAGE(1) 5 minutes, room temperature
SUBSTAGE(2) 12 hours, 35 deg C

STAGE(2)
RCT A **98-85-1**, B 7476-81-5
RGT E 865-47-4 t-BuOK, F 497-19-8 Na2CO3
CAT **470688-18-7** Ruthenium, dicarbonylchloro[(1,2,3,4,5-η)-1-[(1-methylethyl)amino]-2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl]-
SOL 109-99-9 THF

CON 3 days, 25 deg C

PRO C **161024-76-6**
NTE optimization study, optimized on solvent, **stereoselective**, stereoselectivity increased slightly with other acyl donor(TFEB), biotransformation, enzymic

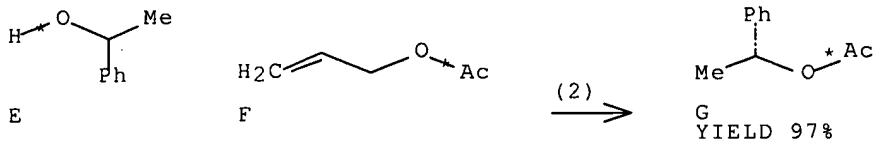
REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L118 ANSWER 6 OF 24 CASREACT COPYRIGHT 2007 ACS on STN DUPLICATE 6
ACCESSION NUMBER: 137:311016 CASREACT Full-text
TITLE: Aminocyclopentadienyl ruthenium chloride: Catalytic racemization and dynamic kinetic resolution of alcohols at ambient temperature
AUTHOR(S): **Choi, Jun Ho**; Kim, Yu Hwan; Nam, Se Hyun; Shin, Seung Tae; **Kim, Mahn-Joo**; **Park, Jaiwook**
CORPORATE SOURCE: National Research Laboratory of Chirotechnology Department of Chemistry Division of Molecular and Life Sciences, Pohang University of Science and Technology (POSTECH), Pohang, 790-784, S. Korea
SOURCE: Angewandte Chemie, International Edition (2002), 41(13), 2373-2376
CODEN: ACIEF5; ISSN: 1433-7851
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English

got it good date

AB Novel racemization catalyst is prepared, [RuCl(CO)2(η5-cyclo- C5Ph4NHCHMe2)] (1), which improves dramatically the ruthenium-enzyme tandem dynamic kinetic resolution (DKR) of secondary alcs. The DKR proceeds at room temperature with isopropenyl acetate as an acyl donor and requires less lipase than with racemization catalysts described earlier. The structure of 1 was determined by x-ray diffraction.

RX(2) OF 12 E + F ===> G



E F G
YIELD 97%

RX(2) RCT E **98-85-1**, F 591-87-7
RGT H 497-19-8 Na2CO3
PRO G **16197-92-5**
CAT **470688-18-7** Ruthenium, dicarbonylchloro[(1,2,3,4,5-η)-1-[(1-methylethyl)amino]-2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl]-, 865-47-4 t-BuOK, 9001-62-1 Lipase
SOL 108-88-3 PhMe
NTE **stereoselective**, >99% ee, enzymic, 25°, 30 h under argon

REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L118 ANSWER 7 OF 24 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 140:405582 CASREACT Full-text
TITLE: Method for the preparation of chiral hydroxy esters by enzyme/metal multi-catalysis
INVENTOR(S): **Kim, Mahn-joo; Park, Jai-wook;** Han, Min-young; Choi, Min-young; **Choi, Yoon-kyung;** Lee, Jae-kwan
PATENT ASSIGNEE(S): Postech Foundation, S. Korea
SOURCE: PCT Int. Appl., 21 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

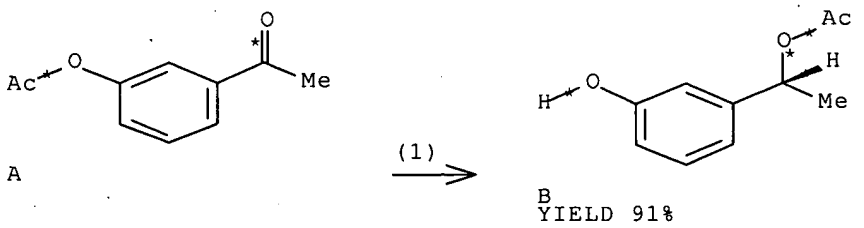
got it. good date

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004039998	A1	20040513	WO 2003-KR1437	20030721
W: CA, CN, IN, JP, US				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR				
KR 2004038176	A	20040508	KR 2002-67058	20021031

PRIORITY APPLN. INFO.: KR 2002-67058 20021031
OTHER SOURCE(S): MARPAT 140:405582

AB The invention provides a process for preparing a chiral hydroxy ester by reacting a compound having both a ketone group and an acyloxy group in a mol. with a hydrogen donor which reduces the ketone group into an hydroxyl group; a metal complex, which catalyzes both the reduction of the ketone and racemization reaction of produced hydroxy group; and an enzyme, which catalyzes enantioselective acyl transfer in an organic solvent.

RX(1) OF 8 **A** ===> **B**



RX(1) RCT A **2454-35-5**

STAGE(1)
CAT 9001-62-1 Lipase, **104439-77-2** Ruthenium, tetracarbonyl-μ-hydro[(1,2,3,4,5-η)-1-hydroxylato-2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl][(1,2,3,4,5-η)-1-hydroxy-2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl]di-

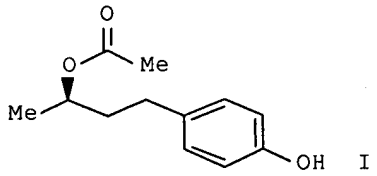
SOL 108-88-3 PhMe
CON room temperature

STAGE(2)
RGT C 1333-74-0 H2
CON 72 hours, room temperature

PRO B **490031-20-4**
NTE biotransformation, enzymic, **stereoselective**, Pseudomonas cepacia lipase/Candida antarctica lipase/Candida rugosa lipase used

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

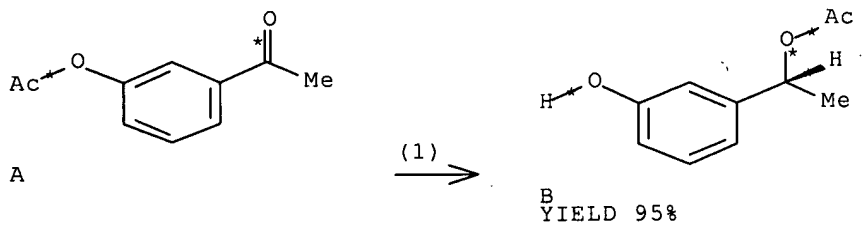
L118 ANSWER 8 OF 24 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 138:122426 CASREACT Full-text
TITLE: Asymmetric Transformations of Acyloxyphenyl Ketones by Enzyme-Metal Multicatalysis
AUTHOR(S): **Kim, Mahn-Joo**; Choi, Min Young; Han, Min Young; **Choi, Yoon Kyung**; Lee, Jae Kwan; **Park, Jaiwook**
CORPORATE SOURCE: National Research Laboratory of Chirotechnology, Department of Chemistry, Division of Molecular and Life Sciences, Pohang University of Science and Technology, Kyongbuk, 790-784, S. Korea
SOURCE: Journal of Organic Chemistry (2002), 67(26), 9481-9483
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

AB A multipathway process comprising several enzyme- and metal-catalyzed reactions has been explored for the asym. transformations of acyloxyphenyl ketones to optically active hydroxyphenyl alcs. in the ester forms, e.g., I. The process comprises nine component reactions in three pathways, all of which take place by the catalytic actions of only two catalysts, a lipase and a ruthenium complex. The synthetic reactions were carried out on 0.2-0.6 mmol scales for eight different substrates under an atmospheric of hydrogen (1 atm) in toluene at 70 °C for 3 days. In most cases, the yields were high (92-96%) and the optical purities were excellent (96-98% ee). This work thus has demonstrated that enzyme-metal multicatalysis has great potential as a new methodol. for asym. transformations.

RX(1) OF 8 A ===> B



RX(1) RCT A **2454-35-5**
RGT C 1333-74-0 H2
PRO B **490031-20-4**
CAT **104439-77-2** Ruthenium, tetracarbonyl-μ-hydro[(1,2,3,4,5-η)-1-hydroxylato-2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl][(1,2,3,4,5-η)-1-hydroxy-2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl]di-, 9001-62-1 Lipase
SOL 108-88-3 PhMe
CON 3 days, 70 deg C
NTE biotransformation, **stereoselective**, lipase PS-D used

REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L118 ANSWER 9 OF 24 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 134:310984 CASREACT Full-text
TITLE: Preparation of chiral esters
INVENTOR(S): **Park, Jai Wook; Kim, Mahn-joo;** Koh, Jeong Hwan; Jung, Hyun Min
PATENT ASSIGNEE(S): Samsung Fine Chemicals Co., Ltd., S. Korea; Pohang University of Science and Technology
SOURCE: PCT Int. Appl., 20 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

didn't get it.

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001028971	A1	20010426	WO 2000-KR1171	20001018
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2387950	A1	20010426	CA 2000-2387950	20001018
AU 2001010589	A	20010430	AU 2001-10589	20001018
KR 2001040122	A	20010515	KR 2000-61351	20001018
EP 1226105	A1	20020731	EP 2000-971840	20001018

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL

JP 2003512035 T 20030402 JP 2001-531776 20001018
PRIORITY APPLN. INFO.: KR 1999-45041 19991018
WO 2000-KR1171 20001018
OTHER SOURCE(S): MARPAT 134:310984

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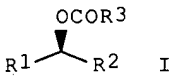
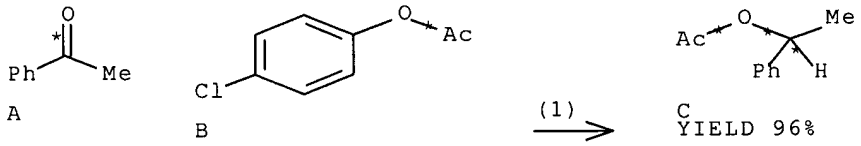


I

AB Title esters [I; R1-R3 = (cyclo)alkyl, aryl, etc.] were prepared from R1COR2 in the presence of a Ru complex, a lipase, a hydride donor, and an acyl donor wherein unacylated alkanol enantiomer is racemized providing for complete conversion.

RX(1) OF 7 **A** + B ===> **C**



A B (1) C YIELD 96%

RX(1) RCT A **98-86-2**

STAGE(1)
RGT D 121-44-8 Et3N, E 108-82-7 4-Heptanol, 2,6-dimethyl-, F 9001-62-1 Lipase
CAT **52462-29-0** Ruthenium, di-μ-chlorodichlorobis[(1,2,3,4,5,6-η)-1-methyl-4-(1-methylethyl)benzene]di-
SOL 75-09-2 CH2Cl2

STAGE(2)
RCT B 876-27-7

PRO C **93-92-5**
NTE enzymic, biotransformation, **stereoselective**
REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

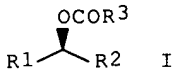
L118 ANSWER 10 OF 24 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 134:310983 CASREACT Full-text
TITLE: Preparation of chiral esters
INVENTOR(S): **Park, Jai Wook; Kim, Mahn-joo;**

Koh, Jeong Hwan; Jung, Hyun Min
PATENT ASSIGNEE(S): Samsung Fine Chemicals Co., Ltd., S. Korea; Pohang University of Science and Technology
SOURCE: PCT Int. Appl., 23 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

got it.

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001028970	A1	20010426	WO 2000-KR1170	20001018
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2387949	A1	20010426	CA 2000-2387949	20001018
AU 2001010588	A	20010430	AU 2001-10588	20001018
KR 2001040121	A	20010515	KR 2000-61350	20001018
EP 1228033	A1	20020807	EP 2000-971839	20001018
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
JP 2003512034	T	20030402	JP 2001-531775	20001018
US 6753443	B1	20040622	US 2001-786276	20010302
PRIORITY APPLN. INFO.:			KR 1999-45040	19991018
			WO 2000-KR1170	20001018

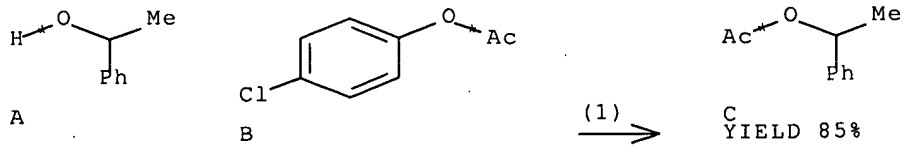
OTHER SOURCE(S): MARPAT 134:310983
GI



I

AB Title esters [I; R1-R3 = (cyclo)alkyl, aryl, etc.] were prepared from racemic alkanols in the presence of a Ru complex, a lipase, and an acyl donor wherein unacylated alkanol enantiomer is racemized providing for complete conversion.

RX(1) OF 6 A + B ===> C

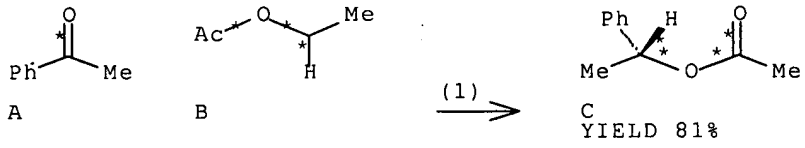


RX(1) RCT A **98-85-1**, B 876-27-7
RGT D 121-44-8 Et3N
PRO C **93-92-5**
CAT **99897-61-7** Ruthenium, chloro[(1,2,3,3a,7a-η)-1H-inden-1-yl]bis(triphenylphosphine)-
SOL 75-09-2 CH2Cl2
NTE **STEREOSELECTIVE**, LIPASE USED
REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L118 ANSWER 11 OF 24 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 133:237398 CASREACT Full-text
TITLE: Practical Ruthenium/Lipase-Catalyzed Asymmetric Transformations of Ketones and Enol Acetates to Chiral Acetates
AUTHOR(S): Jung, Hyun M.; Koh, Jeong H.; **Kim, Mahn-Joo**; **Park, Jaiwook**
CORPORATE SOURCE: Department of Chemistry Division of Molecular Life Science, Pohang University of Science and Technology (POSTECH), Pohang, 790-784, S. Korea
SOURCE: Organic Letters (2000), 2(16), 2487-2490
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Ketones were asym. transformed to chiral acetates by one-pot processes using a lipase and an achiral ruthenium complex under 1 atm of hydrogen gas in Et acetate. Mol. hydrogen was also effective for the transformation of enol acetates to chiral acetates without addnl. acyl donors with the same catalyst system.

I got it.

RX(1) OF 18 **A** + B ===> C



A B C
YIELD 81%

RX(1) RCT A **98-86-2**, B 141-78-6

STAGE(1)
RGT D 9001-62-1 Lipase
SOL 141-78-6 AcOEt

STAGE(2)
RGT E 1333-74-0 H2
CAT **104439-77-2** Ruthenium, tetracarbonyl-μ-hydro[(1,2,3,4,5-η)-1-hydroxylato-2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl][(1,2,3,4,5-η)-1-hydroxy-

2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl]di-

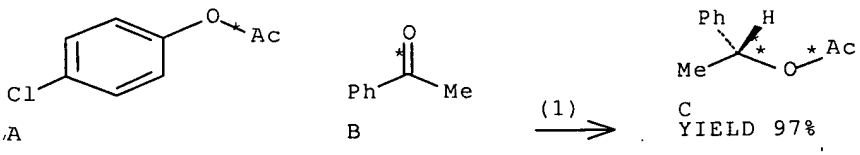
PRO C **16197-92-5**
NTE **STEREOSELECTIVE**
REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L118 ANSWER 12 OF 24 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 132:222047 CASREACT Full-text
TITLE: Concerted Catalytic Reactions for Conversion of Ketones or Enol Acetates to Chiral Acetates
AUTHOR(S): Jung, Hyun M.; Koh, Jeong H.; **Kim, Mahn-Joo**; **Park, Jaiwook**
CORPORATE SOURCE: Department of Chemistry and Division of Molecular & Life Science, Pohang University of Science and Technology (POSTECH), Pohang, 790-784, S. Korea
SOURCE: Organic Letters (2000), 2(3), 409-411
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

got it.

AB Enol acetates or ketones asym. transformed to chiral acetates in high yields with high optical purities through multistep reactions catalyzed by a lipase and a ruthenium complex. 2,6-Dimethyl-4-heptanol was chosen as a suitable hydrogen donor, and 4-chlorophenyl acetate was used as an acyl donor for the conversion of ketones.

RX(1) OF 16 A + B ===> C



RX(1) RCT A 876-27-7, B **98-86-2**
RGT D 9001-62-1 Lipase
PRO C **16197-92-5**
CAT **104439-77-2** Ruthenium, tetracarbonyl-μ-hydro[(1,2,3,4,5-η)-1-hydroxylato-2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl][(1,2,3,4,5-η)-1-hydroxy-2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl]di-
SOL 108-88-3 PhMe
NTE **stereoselective**, ultrasound to increase dispersion in suspension, biotransformation, Novozym 435 used
REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L118 ANSWER 13 OF 24 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 131:286217 CASREACT Full-text
TITLE: Enzymatic resolution of secondary alcohols coupled

with ruthenium-catalyzed racemization without hydrogen mediator

AUTHOR(S): Koh, Jeong Hwan; Jung, Hyun Min; **Kim**, **Mahn-Joo** ; **Park**, **Jaiwook**

CORPORATE SOURCE: Department of Chemistry and Center for Biofunctional Molecules, Pohang University of Science and Technology (POSTECH), Pohang, 790-784, S. Korea

SOURCE: Tetrahedron Letters (1999), 40(34), 6281-6284
CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER: Elsevier Science Ltd.

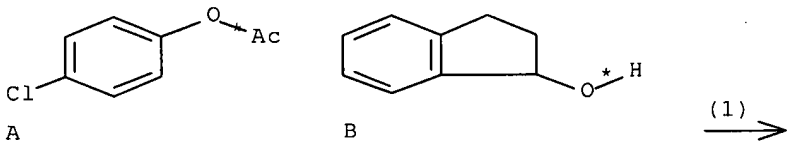
DOCUMENT TYPE: Journal

LANGUAGE: English

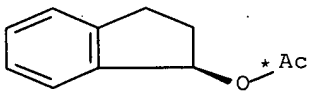
got it.

AB (η5-Indenyl)RuCl(PPh3)2 was found to catalyze the racemization of secondary alcs. in the presence of triethylamine and oxygen. Unlike previously reported metal-catalyzed racemization, ketones were not required as hydrogen mediators in our process. The Ru-catalyzed racemization was coupled with enzymic acetylation for the dynamic kinetic resolution of secondary alcs. to give chiral acetates in good yields (60-98%) with high enantioselectivities (82-99% ee). For example, chloro(η5-indenyl)bis(triphenylphosphine)ruthenium-catalyzed racemization of (±)-1-phenylethanol coupled with lipase-catalyzed acetylation gave (R)-1-phenylethanol acetate in 85% yield (96% enantiomeric excess).

RX(1) OF 6 A + B ===> C



A B

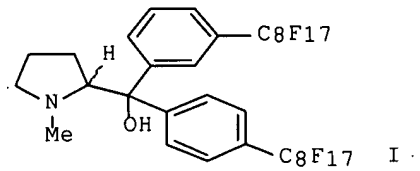


C
YIELD 88%

RX(1) RCT A 876-27-7, B 6351-10-6
RGT D 121-44-8 Et3N, E 7782-44-7 O2
PRO C 879-35-6
CAT 9001-62-1 Lipase, **99897-61-7** Ruthenium, chloro[(1,2,3,3a,7a-η)-1H-inden-1-yl]bis(triphenylphosphine)-
SOL 75-09-2 CH2Cl2
CON 43 hours, 60 deg C
NTE biotransformation, enzymic, **stereoselective**, ee 82%, Pseudomonas cepacia lipase enzyme used, dynamic kinetic resolution

REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L118 ANSWER 14 OF 24 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:101854 CAPLUS Full-text
DOCUMENT NUMBER: 142:336082
TITLE: Asymmetric diethyl- and diphenylzinc additions to aldehydes by using a fluorine-containing **chiral** amino **alcohol**: A striking temperature effect on the enantioselectivity, a minimal amino **alcohol** loading, and an efficient recycling of the amino **alcohol**
AUTHOR(S): **Park, Jin Kyoon; Lee, Hong Geun;** Bolm, Carsten; Kim, B. Moon
CORPORATE SOURCE: School of Chemistry, Seoul National University, Seoul, 151-747, S. Korea
SOURCE: Chemistry--A European Journal (2005), 11(3), 945-950
CODEN: CEUJED; ISSN: 0947-6539
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 142:336082
ED Entered STN: 07 Feb 2005
GI



I

AB A chiral pyrrolidinylmethanol derivative containing perfluoro-ponytails I was prepared from (S)-proline. The use of this perfluoro-substituted amino alc. in catalytic asym. addns. of organozinc reagents to aldehydes affords products with high enantioselectivities in both pure hexane and a mixture of hexane and FC-72 (perfluorohexane). Enantiomeric excesses up to 94 and 88% ee have been achieved in Et2Zn and Ph2Zn addns., resp. For the reactions in the biphasic solvent system a striking temperature effect was observed Thus, when the temperature was raised from 0 to 40°C the ee value of the product increased from 81 to 92%. Furthermore, the catalyst loading could be remarkably low, and with only 0.1 mol% of amino alc. 5 a product with 90% ee was obtained in the Et2Zn addition to benzaldehyde in hexane. The perfluoro-ligand was easily recovered by simple phase separation, and until the ninth repetition its reuse proceeded without significant loss of enantioselectivity and reactivity.
CC 25-7 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 34
ST aryl aldehyde diorganozinc asym addn reaction fluorous amino **alc** ; **chiral** fluorous amino **alc** asym addn catalyst; benzyl **alc** stereoselective prepn
IT Aldehydes, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(aromatic; stereoselective preparation of benzylic **alcs**. via fluorous **chiral** amino **alc**. catalyzed asym. addition reaction of

diorganozincs with arylaldehydes)
IT Alcohols, preparation
RL: SPN (Synthetic preparation); PREP (Preparation)
(benzyl, **chiral**; stereoselective preparation of benzylic **alcs**. via fluorous **chiral** amino **alc**. catalyzed asym. addition reaction of diorganozincs with arylaldehydes)
IT Alcohols, preparation
RL: CAT (Catalyst use); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(**chiral**, amino, fluorous; stereoselective preparation of benzylic **alcs**. via fluorous **chiral** amino **alc**. catalyzed asym. addition reaction of diorganozincs with arylaldehydes)
IT Partition
(fluorous; partition coefficient evaluation and stereoselective preparation of benzylic **alcs**. via fluorous **chiral** amino **alc**. catalyzed asym. addition reaction of diorganozincs with arylaldehydes)
IT Asymmetric synthesis and induction
(stereoselective preparation of benzylic **alcs**. via fluorous **chiral** amino **alc**. catalyzed asym. addition reaction of diorganozincs with arylaldehydes)
IT Addition reaction
Addition reaction catalysts
(stereoselective; stereoselective preparation of benzylic **alcs**. via fluorous **chiral** amino **alc**. catalyzed asym. addition reaction of diorganozincs with arylaldehydes)
IT 848784-93-0P
RL: CAT (Catalyst use); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(partition coefficient; partition coefficient evaluation and stereoselective preparation of benzylic **alcs**. via fluorous **chiral** amino **alc**. catalyzed asym. addition reaction of diorganozincs with arylaldehydes)
IT 110529-22-1
RL: CAT (Catalyst use); USES (Uses)
(stereoselective preparation of benzylic **alcs**. via fluorous **chiral** amino **alc**. catalyzed asym. addition reaction of diorganozincs with arylaldehydes)
IT 100-52-7, Benzaldehyde, reactions 104-55-2, Cinnamaldehyde 104-88-1, p-Chlorobenzaldehyde, reactions 106-37-6, 1,4-Dibromobenzene 123-11-5, p-Methoxybenzaldehyde, reactions 507-63-1, Perfluorooctyl iodide 557-20-0, Diethylzinc 1078-58-6, Diphenylzinc 93423-88-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(stereoselective preparation of benzylic **alcs**. via fluorous **chiral** amino **alc**. catalyzed asym. addition reaction of diorganozincs with arylaldehydes)
IT 848784-90-7P 848784-91-8P 848784-92-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(stereoselective preparation of benzylic **alcs**. via fluorous **chiral** amino **alc**. catalyzed asym. addition reaction of diorganozincs with arylaldehydes)
IT 613-87-6P 73854-04-3P 73890-73-0P 88765-29-1P 101402-04-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(stereoselective preparation of benzylic **alcs**. via fluorous **chiral** amino **alc**. catalyzed asym. addition reaction of diorganozincs with arylaldehydes)
REFERENCE COUNT: 47 THERE ARE 47 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L118 ANSWER 15 OF 24 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:452908 CAPLUS Full-text
DOCUMENT NUMBER: 143:171348
TITLE: Dynamic kinetic resolutions and asymmetric transformations by enzyme-metal combo catalysis
AUTHOR(S): **Kim, Mahn-Joo**; Ahn, Yangsoo; **Park, Jaiwook**
CORPORATE SOURCE: National Research Laboratory of Chirotechnology and Department of Chemistry, Division of Molecular and Life Sciences, Pohang University of Science and Technology, Kyongbuk, 790-784, S. Korea
SOURCE: Bulletin of the Korean Chemical Society (2005), 26(4), 515-522
CODEN: BKCSDE; ISSN: 0253-2964
PUBLISHER: Korean Chemical Society
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English
ED Entered STN: 27 May 2005
AB A review. Enzyme-metal combo catalysis is described as a useful methodol. for the synthesis of optically active compds. The key point of the method is the use of enzyme and metal in combination as the catalysts for the complete transformation of racemic substrates to single enantiomeric products through dynamic kinetic resolution (DKR). In this approach, enzyme acts as an enantioselective resolving catalyst and metal does as a racemizing catalyst for the efficient DKR. Three kinds of enzyme-metal combinations - lipase-ruthenium, subtilisin-ruthenium, and lipase-palladium - have been developed as the catalysts for the DKRs of racemic alcs., esters, and amines. The scope of the combination catalysts can be extended to the asym. transformations of ketones, enol acetates, and ketoximes via the DKRs. In most cases studied, enzyme-metal combo catalysis provided enantiomerically-enriched products in high yields.
CC 16-0 (Fermentation and Bioindustrial Chemistry)
IT **Resolution (separation)**
(enzymic; **dynamic kinetic** resolns. and asym. transformations by enzyme-metal combo catalysis)
REFERENCE COUNT: 66 THERE ARE 66 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L118 ANSWER 16 OF 24 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:236729 CAPLUS Full-text
DOCUMENT NUMBER: 140:433486
TITLE: Fluorometric assay protocol for protease-catalyzed transesterification reactions in organic solvents
AUTHOR(S): Han, Min Su; Jung, Sang Oh; **Kim, Mahn-Joo**; **Kim, Dong H.**
CORPORATE SOURCE: Center for Integrated Molecular Systems, and National Research Laboratory of Chirotechnology, Department of Chemistry, Division of Molecular and Life Sciences, Pohang University of Science and Technology, Pohang, 790-784, S. Korea
SOURCE: Journal of Organic Chemistry (2004), 69(8), 2853-2855
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 23 Mar 2004
AB A fluorometric assay protocol for a subtilisin-catalyzed transesterification reaction in hexane has been developed. The method makes use of a Michael

acceptor that forms a fluorescent adduct with thiophenol, one of the products generated in the transesterification reaction. The method may be employed for screening a biocatalyst useful for transesterification reactions in organic solvents and for optimizing the transesterification reaction conditions. Thus, this protocol takes advantage of the facile Michael acceptor properties of a com. available dye, 7-diethylamino-3-(4'-maleimidylphenyl)-4-methylcoumarin, with benzenethiol formed in the above transesterification, thus giving a highly fluorescent product.

CC 80-5 (Organic Analytical Chemistry)
Section cross-reference(s): 25

IT Fluorescent substances
Michael reaction
Transesterification
(fluorometric assay protocol for protease-catalyzed transesterification of **chiral** (carbonylamino)benzenepropanethioic acid esters with **alcs**. and capture of benzenethiol with (diethylamino)(maleimidylphenyl)(methyl)coumarin)

IT Alcohols, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(fluorometric assay protocol for protease-catalyzed transesterification of **chiral** (carbonylamino)benzenepropanethioic acid esters with **alcs**. and capture of benzenethiol with (diethylamino)(maleimidylphenyl)(methyl)coumarin)

IT 9014-01-1, Subtilisin
RL: CAT (Catalyst use); USES (Uses)
(Carlsberg; fluorometric assay protocol for protease-catalyzed transesterification of **chiral** (carbonylamino)benzenepropaneth ioic acid esters with **alcs**. and capture of benzenethiol with (diethylamino)(maleimidylphenyl)(methyl)coumarin)

IT 691413-66-8P
RL: BPN (Biosynthetic preparation); PNU (Preparation, unclassified); BIOL (Biological study); PREP (Preparation)
(fluorometric assay protocol for protease-catalyzed transesterification of **chiral** (carbonylamino)benzenepropanethioic acid esters with **alcs**. and capture of benzenethiol with (diethylamino)(maleimidylphenyl)(methyl)coumarin)

IT 108-98-5P, Benzenethiol, reactions
RL: BPN (Biosynthetic preparation); RCT (Reactant); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(fluorometric assay protocol for protease-catalyzed transesterification of **chiral** (carbonylamino)benzenepropanethioic acid esters with **alcs**. and capture of benzenethiol with (diethylamino)(maleimidylphenyl)(methyl)coumarin)

IT 9004-07-3, α-Chymotrypsin 37259-58-8, Serine protease
RL: CAT (Catalyst use); USES (Uses)
(fluorometric assay protocol for protease-catalyzed transesterification of **chiral** (carbonylamino)benzenepropanethioic acid esters with **alcs**. and capture of benzenethiol with (diethylamino)(maleimidylphenyl)(methyl)coumarin)

IT 71-23-8, 1-Propanol, reactions 811-51-8, Ethanethiol sodium salt 1161-13-3 2018-61-3 76877-33-3, 7-(Diethylamino)-3-(4'-maleimidylphenyl)-4-methylcoumarin
RL: RCT (Reactant); RACT (Reactant or reagent)
(fluorometric assay protocol for protease-catalyzed transesterification of **chiral** (carbonylamino)benzenepropanethioic acid esters with **alcs**. and capture of benzenethiol with (diethylamino)(maleimidylphenyl)(methyl)coumarin)

IT 2075-55-0P, (αS)-α-[[(Phenylmethoxy)carbonyl]amino]benzeneprop anethioic acid S-phenyl ester 60718-38-9P, (αS)-α-

[[(Phenylmethoxy)carbonyl]amino]benzenepropanethioic acid S-ethyl ester 79128-07-7P, (αS)-α-(Acetylamino)benzenepropanethioic acid S-phenyl ester 99685-32-2P, (αS)-α-(Acetylamino)benzenepropanethioic acid S-ethyl ester
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(fluorometric assay protocol for protease-catalyzed transesterification of **chiral** (carbonylamino)benzenepropanethioic acid esters with **alcs**. and capture of benzenethiol with (diethylamino)(maleimidylphenyl)(methyl)coumarin)

IT 110-54-3, Hexane, uses
RL: NUU (Other use, unclassified); USES (Uses)
(fluorometric assay protocol for protease-catalyzed transesterification of **chiral** (carbonylamino)benzenepropanethioic acid esters with **alcs**. in organic solvents and capture of benzenethiol with (diethylamino)(maleimidylphenyl)(methyl)coumarin)

REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L118 ANSWER 17 OF 24 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:96174 CAPLUS Full-text
DOCUMENT NUMBER: 140:4084
TITLE: Dynamic kinetic resolutions and asymmetric transformations by enzymes coupled with metal catalysis. [Erratum to document cited in CA138:186421]
AUTHOR(S): **Kim, Mahn-Joo**; Ahn, Yangsoo; **Park, Jaiwook**
CORPORATE SOURCE: Division of Molecular and Life Sciences, Department of Chemistry, National Research Laboratory of Chirotechnology, Pohang University of Science and Technology, kyungbuk, 790-784, S. Korea
SOURCE: Current Opinion in Biotechnology (2003), 14(1), 131
CODEN: CUOBE3; ISSN: 0958-1669
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English
got it.
ED Entered STN: 07 Feb 2003
AB A review. The wrong legend was incorporated with Figure 6; the corrected version of the figure and legend is given. In the section on "Asym. reductive acetylation of ketoximes" the correct definition of Pd/C should have been given as palladium on carbon.
CC 16-0 (Fermentation and Bioindustrial Chemistry)
Section cross-reference(s): 7, 21
IT **Resolution (separation)**
(enzymic, **kinetic; dynamic kinetic** resolns. and asym. transformations by enzymes coupled with metal catalysis (Erratum))

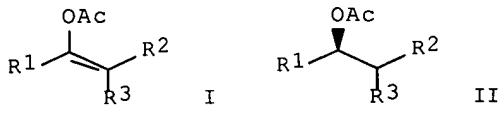
L118 ANSWER 18 OF 24 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:931631 CAPLUS Full-text
DOCUMENT NUMBER: 138:186421
TITLE: Dynamic kinetic resolutions and asymmetric transformations by enzymes coupled with metal catalysis
AUTHOR(S): **Kim, Mahn-Joo**; Ahn, Yangsoo; **Park, Jaiwook**
CORPORATE SOURCE: Division of Molecular and Life Sciences, Department of Chemistry, National Research Laboratory of Chirotechnology, Pohang University of Science and Technology, Kyungbuk, 790-784, S. Korea

SOURCE: Current Opinion in Biotechnology (2002), 13(6), 578-587
CODEN: CUOBE3; ISSN: 0958-1669
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English
ED Entered STN: 09 Dec 2002
AB A review, with refs. The combination of enzyme and metal catalysis is described as a useful method for the synthesis of optically active compds. A key feature of this new methodol. is the use of metal catalysts for the in situ racemization of enzymically unreactive enantiomers in the enzymic resolution of racemic substrates. So far, two combinations - lipase-ruthenium and lipase-palladium - have been developed for the efficient dynamic kinetic resolution of alcs. and amines. The use of these combinations has also been extended to catalysis of the asym. transformation of ketones, their enol acetates, and ketoximes. In most cases, enzyme-metal combination catalysis has provided good yields and high optical purities. Coupled enzyme-metal catalysis is a new approach for the dynamic kinetic resolution and asym. transformations and provides a useful alternative to conventional chemical or enzymic methods.
CC 16-0 (Fermentation and Bioindustrial Chemistry)
Section cross-reference(s): 7, 21
IT **Resolution (separation)**
(enzymic, **kinetic; dynamic kinetic** resolns. and asym. transformations by enzymes coupled with metal catalysis)
REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L118 ANSWER 19 OF 24 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:416874 CAPLUS Full-text
DOCUMENT NUMBER: 135:19231
TITLE: Stereoselective method for preparing chiral esters from alkenyl esters via ruthenium catalyzed reduction and enzymic resolution
INVENTOR(S): **Park, Jai Wook; Kim, Mahn-joo;** Koh, Jeong Hwan; Jung, Hyun Min
PATENT ASSIGNEE(S): Samsung Fine Chemicals Co., Ltd., S. Korea; Pohang University of Science and Technology
SOURCE: PCT Int. Appl., 19 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001040157	A1	20010607	WO 2000-KR1169	20001018
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2393336	A1	20010607	CA 2000-2393336	20001018
AU 2001010587	A5	20010612	AU 2001-10587	20001018
KR 2001060160	A	20010706	KR 2000-61352	20001018

EP 1237837 A1 20020911 EP 2000-971838 20001018
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL
JP 2003515336 T 20030507 JP 2001-541847 20001018
US 2001012898 A1 20010809 US 2000-726412 20001201
US 6475773 B2 20021105
PRIORITY APPLN. INFO.: KR 1999-54472 A 19991202
WO 2000-KR1169 W 20001018
OTHER SOURCE(S): CASREACT 135:19231; MARPAT 135:19231
ED Entered STN: 08 Jun 2001
GI



AB A method for preparing optically pure chiral esters I (R1, R2 and R3 = independently (un)substituted alkyl, aryl or cycloalkyl group and R1 and R2, R1 and R3, and R2 and R3 can form a cyclic ring; substituent may be halogen or cyano group) in high yield from alkenyl esters via ruthenium catalyzed reduction/racemization with successive enzymic resolution is diclosed. For example, II was synthesized in 89% yield (98% enantiomeric excess) by mixing 1-phenylethenyl acetate with 2,6-dimethylheptan-4-ol, a ruthenium catalyst, and Novozym 435 followed by heating under Argon with subsequent chromatog. purification The chiral esters obtained can be used as synthetic intermediates for preparing various chiral compds., chiral pharmaceutical drugs (e.g. Atorvastatin and Agenerase) or chiral agrochems. (e.g. L-Carnitine).

IC ICM C07C051-16
ICS C12P007-00
CC 21-2 (General Organic Chemistry)
Section cross-reference(s): 29

IT Esters, preparation
RL: BPN (Biosynthetic preparation); IMF (Industrial manufacture); BIOL (Biological study); PREP (Preparation)
(**chiral**; stereoselective method for preparing **chiral** esters from alkenyl esters via ruthenium catalyzed reduction and enzymic resolution of racemic **alc**. intermediate)

IT Resolution (separation)
(enzymic, kinetic; stereoselective method for preparing **chiral** esters from alkenyl esters via ruthenium catalyzed reduction and enzymic resolution of racemic **alc**. intermediate)

IT Burkholderia cepacia
Candida antarctica
(lipase from; stereoselective method for preparing **chiral** esters from alkenyl esters via ruthenium catalyzed reduction and enzymic resolution of racemic **alc**. intermediate)

IT Hydrogenation
Stereoselective synthesis
(stereoselective method for preparing **chiral** esters from alkenyl esters via ruthenium catalyzed reduction and enzymic resolution of racemic **alc**. intermediate)

IT 54712-18-4P 58396-29-5P 68567-23-7P 115729-61-8P 129098-41-5P 137408-28-7P 137408-29-8P

RL: BPN (Biosynthetic preparation); IMF (Industrial manufacture); PUR (Purification or recovery); BIOL (Biological study); PREP (Preparation)
(stereoselective method for preparing **chiral** esters from alkenyl esters via ruthenium catalyzed reduction and enzymic resolution of racemic **alc.** intermediate)

IT 9001-62-1, Novozym 435 52462-29-0 104439-77-2
RL: CAT (Catalyst use); USES (Uses)
(stereoselective method for preparing **chiral** esters from alkenyl esters via ruthenium catalyzed reduction and enzymic resolution of racemic **alc.** intermediate)

IT 16197-93-6P
RL: IMF (Industrial manufacture); PREP (Preparation)
(stereoselective method for preparing **chiral** esters from alkenyl esters via ruthenium catalyzed reduction and enzymic resolution of racemic **alc.** intermediate)

IT 2206-94-2, 1-Phenylethenyl acetate 19455-83-5 22390-98-3 22479-32-9 26735-85-3 52789-67-0 260980-77-6 342808-62-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(stereoselective method for preparing **chiral** esters from alkenyl esters via ruthenium catalyzed reduction and enzymic resolution of racemic **alc.** intermediate)

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L118 ANSWER 20 OF 24 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:877563 CAPLUS Full-text
DOCUMENT NUMBER: 142:74253
TITLE: Process for preparation of **chiral** allyl **alcohol**
INVENTOR(S): **Choi, Yun Gyeong**; Huh, Eun A.; Jung, Jae Yun; **Kim, Man Ju**; Lee, Dong Hyeon; Seo, Jong Hwa
PATENT ASSIGNEE(S): Postech Foundation, S. Korea
SOURCE: Repub. Korean Kongkae Taeho Kongbo, No pp. given
CODEN: KRXXA7
DOCUMENT TYPE: Patent
LANGUAGE: Korean
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
KR 2001037656	A	20010515	KR 1999-45308	19991019
PRIORITY APPLN. INFO.:			KR 1999-45308	19991019

ED Entered STN: 22 Oct 2004

AB Provided is a process for producing chiral allyl alc. excellent in optical purity and synthetic yield by using a palladium metal catalyst for racemization of chiral allyl ester and an enzyme for producing the chiral allyl alc. from the racemic allyl ester. The chiral allyl alc. is produced by reacting the allyl ester, more than 5 mol% (based on the allyl ester) of the palladium(0) complex for the racemization of the allyl ester, 0.2-0.8 g (based on the racemic allyl ester of 1 mmol) of lipase for diacylating selectively an enantiomer of the allyl ester, and more than 10 equiv (based on the racemic allyl ester) of an acyl acceptor. The palladium(0) complex is selected from the group consisting of Pd(PPh3)4 and tris(dibenzylidene acetone)dipalladium(0). The acyl acceptor is selected from the group consisting of iso-Pr alc., Pr alc., Bu alc., and pentyl alc.

IC ICM C07C029-00
CC 23-7 (Aliphatic Compounds)
ST **chiral** allyl **alc** prepn palladium catalytic

racemization
IT 107-18-6P, Allyl **alcohol**, preparation
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of **chiral** allyl **alc.**)

L118 ANSWER 21 OF 24 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:412568 CAPLUS Full-text
DOCUMENT NUMBER: 135:152357
TITLE: Lipase/Ruthenium-Catalyzed Dynamic Kinetic Resolution of Hydroxy Acids, Diols, and Hydroxy Aldehydes Protected with a Bulky Group
AUTHOR(S): **Kim**, **Mahn-Joo**; **Choi**, **Yoon Kyung**; Choi, Min Young; **Kim**, **Mi Jung**; **Park**, **Jaiwook**
CORPORATE SOURCE: National Research Laboratory of Chirotechnology Department of Chemistry Division of Molecular and Life Sciences, Pohang University of Science and Technology, Pohang Kyungbuk, 790-784, S. Korea
SOURCE: Journal of Organic Chemistry (2001), 66(13), 4736-4738
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 135:152357
ED Entered STN: 08 Jun 2001
AB The racemic title substrates were modified with bulky protecting groups and then subjected to the lipase/ruthenium-catalyzed dynamic kinetic resolution (DKR). E.g., DKR of MeCH(OH)CH2CO2CH2Ph with Pseudomonas cepacia lipase, a Ru catalyst, and 4-ClC6H4OAc gave (R)-MeCH(OAc)CH2CO2CH2Ph (88% yield, 86 % ee).
CC 21-2 (General Organic Chemistry)
IT **Resolution (separation)**
(**kinetic**; lipase/ruthenium-catalyzed **dynamic kinetic** resolution of hydroxy acids, diols, and hydroxy aldehydes protected with a bulky group)
REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L118 ANSWER 22 OF 24 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2000:455856 CAPLUS Full-text
DOCUMENT NUMBER: 133:222192
TITLE: Dynamic Kinetic Resolution of Allylic Alcohols Mediated by Ruthenium- and Lipase-Based Catalysts
AUTHOR(S): Lee, Donghyun; Huh, Eun A.; **Kim**, **Mahn-Joo**; Jung, Hyun Min; Koh, Jeong Hwan; **Park**, **Jaiwook**
CORPORATE SOURCE: Department of Chemistry Division of Molecular and Life Science, Pohang University of Science and Technology, Pohang Kyungbuk, 790-784, S. Korea
SOURCE: Organic Letters (2000), 2(15), 2377-2379
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 133:222192
ED Entered STN: 07 Jul 2000
AB An enzyme-metal combo reaction has been developed for the dynamic kinetic resolution of allylic alcs. in which racemic substrates are transformed by a lipase and a ruthenium complex in the presence of an acyl donor to allylic acetates of high optical purity in over 80% yield.
CC 21-3 (General Organic Chemistry)
Section cross-reference(s): 16

IT Racemization
Racemization
(catalysts, Ru-catalyzed racemization of **chiral** allylic **alcs.**; synthesis of homochiral allylic acetates via enantioselective enzymic acetylation of racemic allylic **alcs.** and Ru-catalyzed racemization of unreacted substrate)
IT Racemization
(of **chiral** allylic **alcs.**; synthesis of homochiral allylic acetates via enantioselective enzymic acetylation of racemic allylic **alcs.** and Ru-catalyzed racemization of unreacted substrate)
IT Isomerization catalysts
Isomerization catalysts
(racemization catalysts, Ru-catalyzed racemization of **chiral** allylic **alcs.**; synthesis of homochiral allylic acetates via enantioselective enzymic acetylation of racemic allylic **alcs.** and Ru-catalyzed racemization of unreacted substrate)
IT 122-57-6P, 3-Buten-2-one, 4-phenyl- 2550-26-7P, Butan-2-one, 4-phenyl-
RL: BYP (Byproduct); PREP (Preparation)
(side-product in racemization of **chiral** allylic **alcs**.; synthesis of homochiral allylic acetates via enantioselective enzymic acetylation of racemic allylic **alcs.** and Ru-catalyzed racemization of unreacted substrate)
REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L118 ANSWER 23 OF 24 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1999:643342 CAPLUS Full-text
DOCUMENT NUMBER: 132:35316
TITLE: Dynamic Kinetic Resolution of Acyclic Allylic Acetates Using Lipase and Palladium
AUTHOR(S): **Choi, Yoon Kyung**; Suh, Jong Hwa; Lee, Donghyun; Lim, In Taek; Jung, Jae Yoon; **Kim, Mahn-Joo**
CORPORATE SOURCE: Department of Chemistry and Center for Biofunctional Molecules, Pohang University of Science and Technology, Pohang, 790-784, S. Korea
SOURCE: Journal of Organic Chemistry (1999), 64(22), 8423-8424
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 132:35316
ED Entered STN: 11 Oct 1999
AB Racemic allylic acetates MeCH(OAc)CH:CHR (R = Ph, 4-ClC6H4, 4-MeC6H4, 2-furyl, 1-naphthyl) were transformed into single enantiomeric products (R)-MeCH(OH)CH:CHR through lipase-catalyzed transesterification coupled with Pd-catalyzed racemization.
CC 21-2 (General Organic Chemistry)
Section cross-reference(s): 7, 9
IT **Resolution (separation)**
(**kinetic; dynamic kinetic** resolution of acyclic allylic acetates through lipase-catalyzed transesterification coupled with Pd-catalyzed racemization)
REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L118 ANSWER 24 OF 24 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1998:101619 CAPLUS Full-text
DOCUMENT NUMBER: 128:200296

TITLE: Enantioselectivity of heptakis(6-O-alkyldimethylsilyl-2,3-di-O-ethyl)-β-cyclodextrins as chiral stationary phases in capillary gas chromatography

AUTHOR(S): Kim, Byoung Eog; **Kim, Min Kyun**; Ryu, Young Kyun; **Park, Jung Kon**; **Park, Jung Hag**

CORPORATE SOURCE: Research Institute of Industrial Science and Technology, Pohang, 790-330, S. Korea

SOURCE: Analytical Sciences (1997), 13(Suppl., Asianalysis IV), 263-266
CODEN: ANSCEN; ISSN: 0910-6340

PUBLISHER: Japan Society for Analytical Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

ED Entered STN: 20 Feb 1998

AB Four heptakis(6-O-alkyldimethylsilyl-2,3-di-O-ethyl)-β-cyclodextrin (CD) having 6-O-alkyl groups of different chain length, heptakis(6-O-trimethylsilyl-2,3-di-O-ethyl)-β-CD (MTDE-β-CD), heptakis(6-O-ethyldimethylsilyl-2,3-di-O-ethyl)-β-CD (ETDE-β-CD), heptakis(6-O-octyldimethylsilyl-2,3-di-O-ethyl)-β- CD (OTDE-β-CD) and heptakis(6-O-octadecyldimethylsilyl-2,3-di-O- ethyl)-β-CD (ODDE-β-CD), were prepared and effect of the chain length of the 6-O-alkyl moiety on the enantioselectivity of the CD derivs. as chiral stationary phases were compared by measuring separation factors of a range of chiral test compds. in capillary gas chromatog. Enantioselectivity of the CD derivs. is in the order, ETDE-β-CD ≥ MTDE-β-CD > OTDE-β-CD > ODDE-β-CD.

CC 80-4 (Organic Analytical Chemistry)

IT 78-76-2, (±)-2-Bromobutane 80-56-8, (±)-α-Pinene 93-54-9, (±)-1-Phenyl-1-propanol 98-85-1, (±)-sec-Phenethyl **alcohol** 107-81-3, (±)-2-Bromopentane 120-45-6, (±)-1-Phenylethyl propionate 138-86-3, (±)-Limonene 598-32-3, (±)-3-Buten-2-ol 613-87-6, (-)-1-Phenyl-1-propanol 822-67-3, (±)-2-Cyclohexen-1-ol 926-58-9, (-)-trans-3-Penten-2-ol 1072-86-2, (-)-trans-1,2-Cyclohexanediol 1123-85-9, (±)-2-Phenyl-1-propanol 1445-91-6, (-)-sec-Phenethyl **alcohol** 1460-57-7, (±)-trans-1,2-Cyclohexanediol 1517-69-7, (+)-sec-Phenethyl **alcohol** 1565-74-8, (+)-1-Phenyl-1-propanol 1974-04-5, (±)-2-Bromoheptane 2902-96-7, (±)-2-Nitro-1-propanol 3413-44-3, (+)-2-Cyclohexen-1-ol 3899-34-1, (±)-trans-3-Penten-2-ol 5787-32-6, (+)-2-Bromobutane 5787-33-7, (-)-2-Bromobutane 5989-27-5, (+)-Limonene 5989-54-8, (-)-Limonene 6118-13-4, (+)-3-Buten-2-ol 6426-26-2, (-)-2-Cyclohexen-1-ol 7785-26-4, (-)-α-Pinene 7785-70-8, (+)-α-Pinene 19141-40-3, (+)-2-Phenyl-1-propanol 29117-44-0, (-)-2-Bromopentane 29882-58-4, (+)-2-Bromopentane 33447-72-2, (-)-3-Buten-2-ol 35666-69-4, (+)-trans-3-Penten-2-ol 37778-99-7, (-)-2-Phenyl-1-propanol 57794-08-8, (+)-trans-1,2-Cyclohexanediol 107832-32-6, (R)-1-Phenylethyl propionate 117290-46-7, (S)-1-Phenylethyl propionate 130232-91-6, (+)-2-Bromoheptane 130232-92-7, (-)-2-Bromoheptane 192045-60-6, (R)-2-Nitro-1-propanol 192045-61-7, (S)-2-Nitro-1-propanol
RL: ANT (Analyte); PEP (Physical, engineering or chemical process); PRP (Properties); ANST (Analytical study); PROC (Process)
(enantioselectivity of heptakis(6-O-alkyldimethylsilyl-2,3-di-O-ethyl)-β-cyclodextrins as **chiral** stationary phases in capillary GC resolution of)

REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

REACTION SEARCH

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FILE CONTENT:1840 - 28 Jan 2007 VOL 146 ISS 5

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This file contains CAS Registry Numbers for easy and accurate substance
identification.


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L24           1 SEA FILE=REGISTRY ABB=ON  SUBTILISIN/CN
L25           1 SEA FILE=REGISTRY ABB=ON  PROTEINASE/CN
L67       72677 SEA FILE=CASREACT ABB=ON  STEREOSELECTIVE/NTE
L68       30236 SEA FILE=REGISTRY ABB=ON  L14 AND CASREACT/LC
L69        8227 SEA FILE=CASREACT ABB=ON  L68/CAT
L70         267 SEA FILE=CASREACT ABB=ON  L24/CAT OR L25/CAT
L73       76833 SEA FILE=CASREACT ABB=ON  (L69 OR L70 OR L67)
L76             STR
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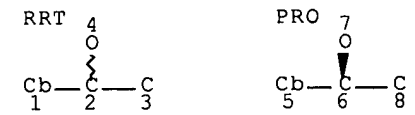


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CONNECT IS E1  RC AT   4
CONNECT IS E3  RC AT   6
DEFAULT MLEVEL IS ATOM
GGCAT   IS UNS  AT   1
GGCAT   IS UNS  AT   5
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS   8

STEREO ATTRIBUTES:
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STEREO DEFAULT ABSOLUTE
NUMBER OF CHIRAL CENTERS IS 1

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  4 O        RRT      7 O        PRO
  6 C        PRO      2 C        RRT
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L122             STR
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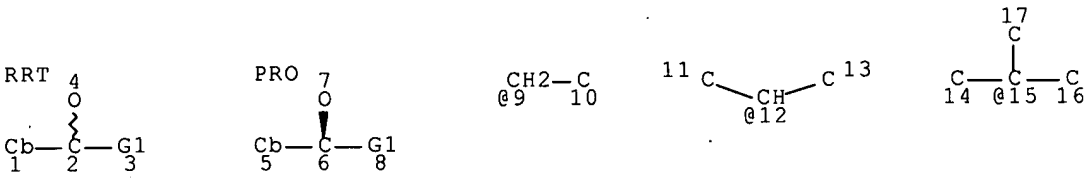


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CONNECT IS E1  RC AT   4
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GGCAT    IS UNS  AT   1
GGCAT    IS UNS  AT   5
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  17

STEREO ATTRIBUTES:
STEREO DEFAULT ABSOLUTE
NUMBER OF CHIRAL CENTERS IS 1

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  6 C        PRO      2 C        RRT
  7 O        PRO      4 O        RRT
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=> d que nos l129; d que nos l130; s l129,l130 not l97
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L67        72677 SEA FILE=CASREACT ABB=ON  STEREOSELECTIVE/NTE
L68        30236 SEA FILE=REGISTRY ABB=ON  L14 AND CASREACT/LC
L69         8227 SEA FILE=CASREACT ABB=ON  L68/CAT
L70          267 SEA FILE=CASREACT ABB=ON  L24/CAT OR L25/CAT
L73        76833 SEA FILE=CASREACT ABB=ON  (L69 OR L70 OR L67)
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L131         17 (L129 OR L130) NOT L97

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L29         226 SEA FILE=CAPLUS ABB=ON  L28(L)L22
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L44       11738 SEA FILE=CAPLUS ABB=ON  RACEMIC/OBI
L45          10 SEA FILE=CAPLUS ABB=ON  L43(L)L44 AND L19 AND (L20 OR L21 OR
                L22 OR L35 OR L41)


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L132         27 (L31 OR L30 OR L39 OR L42 OR L45) NOT L117

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PROCESSING COMPLETED FOR L132
L133          42 DUP REM L131 L132 (2 DUPLICATES REMOVED)
                 ANSWERS '1-17' FROM FILE CASREACT
                 ANSWERS '18-42' FROM FILE CAPLUS

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L133 ANSWER 1 OF 42  CASREACT  COPYRIGHT 2007 ACS on STN DUPLICATE 1
ACCESSION NUMBER:         138:271003  CASREACT  Full-text
TITLE:                    Efficient lipase-catalyzed kinetic resolution and
                          dynamic kinetic resolution of β-hydroxy nitriles.
                          Correction of absolute configuration and
                          transformation to chiral β-hydroxy acids and
                          γ-amino alcohols
AUTHOR(S):                Pamies, Oscar; Backvall, Jan-E.
CORPORATE SOURCE:         Department of Organic Chemistry, Arrhenius Laboratory,
                          Stockholm University, Stockholm, 106 91, Swed.
SOURCE:                   Advanced Synthesis & Catalysis (2002), 344(9), 947-952
                          CODEN: ASCAF7; ISSN: 1615-4150
PUBLISHER:                Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE:            Journal
LANGUAGE:                 English
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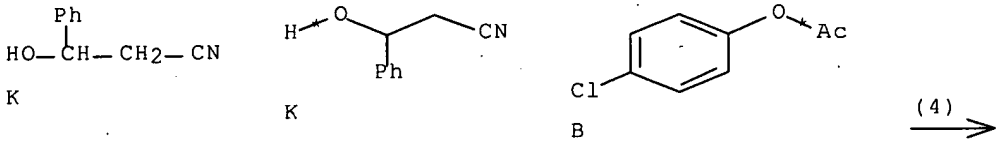
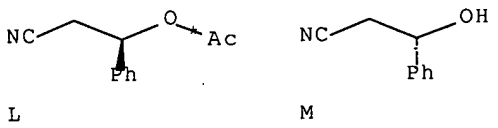
got it

AB Chemoenzymic dynamic kinetic resolution of β-hydroxy nitriles has been carried out using Candida antarctica lipase B and a ruthenium catalyst. The use of a hydrogen source to depress ketone formation in the dynamic kinetic resolution yields the acetates in good yield and high enantioselectivity. It is shown that the ruthenium catalyst and the enzyme can be recycled when used in sep. reactions. Enantiomerically pure β-hydroxy acid derivs. and γ-amino alcs. were prepared from the hydroxy nitriles and acetates. The latter compds. were also used to establish the correct absolute configuration of the hydroxy nitriles and acetates.

RX(4) OF 50 2 **K** + B ===> L + **M**...





RX(4) RCT K **17190-29-3**, B 876-27-7
PRO L 198561-42-1, M **132203-26-0**
CAT 9001-62-1 Lipase, **104439-77-2** Ruthenium, tetracarbonyl-μ-hydro[(1,2,3,4,5-η)-1-hydroxylato-2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl][(1,2,3,4,5-η)-1-hydroxy-2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl]di-
SOL 108-88-3 PhMe
CON 24 hours, 60 deg C
NTE Biotransformation, **enzymic, stereoselective**, kinetic resoln., Candida antarctica lipase B (N-435) present as catalyst

REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

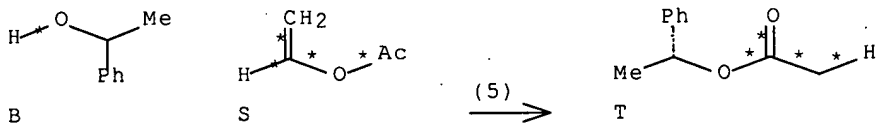
=> d ibib abs fhit 2-17; d ibib ed abs hitind 18-42; fil hom

L133 ANSWER 2 OF 42 CASREACT COPYRIGHT 2007 ACS on STN DUPLICATE 2
ACCESSION NUMBER: 130:266981 CASREACT Full-text
TITLE: Ruthenium- and Enzyme-Catalyzed Dynamic Kinetic Resolution of Secondary Alcohols
AUTHOR(S): Persson, B. Anders; Larsson, Anna L. E.; Le Ray, Mikaeel; Baeckvall, Jan-E.
CORPORATE SOURCE: Departments of Organic Chemistry, Uppsala University, Uppsala, S-751 21, Swed.
SOURCE: Journal of the American Chemical Society (1999),

121(8), 1645-1650
CODEN: JACSAT; ISSN: 0002-7863 opt-21.
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Enzymic resolution of secondary alcs. under substrate racemizing conditions was studied using an immobilized lipase from Candida antarctica in the presence of a Ru catalyst. A specifically designed acyl donor, 4-chlorophenyl acetate, is compatible with both catalysts and resulted in an efficient dynamic kinetic resolution Studies of the reaction in different solvents showed that nonpolar solvents gave the best results. With this process, racemic secondary alcs. were transformed to the corresponding enantiomerically pure acetates, making efficient use of all starting material. In most cases, the reaction proceeded with >99% ee and in good yield.

RX(5) OF 37 ...B + S ===> T



RX(5) RCT B **98-85-1**, S 108-05-4
RGT C 98-86-2 Acetophenone
PRO T **16197-92-5**
CAT **104439-77-2** Ruthenium, tetracarbonyl-μ-hydro[(1,2,3,4,5-η)-1-hydroxylato-2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl][(1,2,3,4,5-η)-1-hydroxy-2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl]di-, 9001-62-1 Lipase
SOL 75-65-0 t-BuOH
CON 17 hours, 70 deg C
NTE **stereoselective**, solid-supported catalyst, **enzymic**, biotransformation, lipase B (Novozyme 435) supported on acrylic resin from Candida antartica used, ee >99%, kinetic resolution

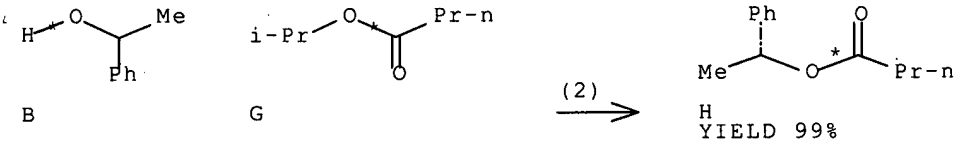
REFERENCE COUNT: 97 THERE ARE 97 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L133 ANSWER 3 OF 42 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 146:7598 CASREACT Full-text
TITLE: Efficient dynamic kinetic resolution of secondary alcohols with a novel tetrafluorosuccinato ruthenium complex
AUTHOR(S): van Nispen, Sjoerd F. G. M.; van Buijtenen, Jeroen; Vekemans, Jef A. J. M.; Meuldijk, Jan; Hulshof, Lumbertus A.
CORPORATE SOURCE: Laboratory of Macromolecular and Organic Chemistry, Eindhoven University of Technology, Eindhoven, 5600 MB, Neth.
SOURCE: Tetrahedron: Asymmetry (2006), 17(15), 2299-2305
CODEN: TASYE3; ISSN: 0957-4166
PUBLISHER: Elsevier Ltd.

DOCUMENT TYPE: Journal
LANGUAGE: English

AB Dynamic kinetic resolution (DKR) of a series of secondary alcs. RCH(OH)Me (R = n-C6H13, Ph, 4-MeOC6H4, 4-F3CC6H4, 2-furyl) has been conducted with a novel dinuclear ruthenium complex, bearing tetrafluorosuccinate and rac-BINAP ligands as the racemization catalyst. Novozym 435 has been used as the enzyme, and iso-Pr butyrate as the acyl donor. The catalyst performed optimally at 70 °C. Typically the reaction reached complete conversion within 1 day with 0.1 mol % of racemization catalyst relative to the substrate. The addition of the ketone corresponding to the substrate stabilizes the active Ru complex and, therefore, increases the rate of the reaction.

RX(2) OF 7 ...**B** + G ===> **H**



RX(2) RCT B **98-85-1**, G 638-11-9
RGT D 584-08-7 K2CO3
PRO H **89378-61-0**
CAT **878999-28-1** Ruthenium, diaquabis[[1,1'-binaphthalene]-2,2'-diylbis[diphenylphosphine-κP]]dicarbonylbis[μ-[tetrafluorobutanedioato(2-)-κO1:κO4]]di-, stereoisomer, 9001-62-1 Lipase
SOL 108-88-3 PhMe
CON 23 hours, 70 deg C, 200 mbar
NTE **enzymic, stereoselective**, >99% ee

REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L133 ANSWER 4 OF 42 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 143:365755 CASREACT Full-text
TITLE: Process for the preparation of enantiomerically enriched esters and alcohols by means of azeotropically dried enzyme compositions
INVENTOR(S): Verzijl, Gerardus Karel Maria
PATENT ASSIGNEE(S): DSM Ip Assets B. V., Neth.
SOURCE: PCT Int. Appl., 32 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005095629	A1	20051013	WO 2005-EP3312	20050325

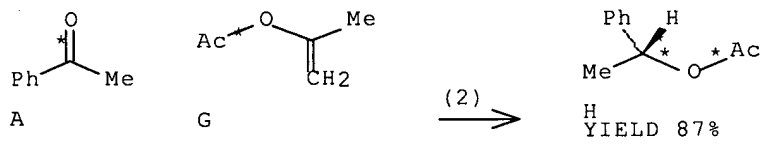
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,

GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM,
SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT,
RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML,
MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: EP 2004-75942 20040329

AB Process for the preparation of an enantiomerically enriched ester, which comprises subjecting a mixture of enantiomers of the corresponding secondary alc., in the presence of an acyl donor, to an enantioselective enzymic conversion, wherein the conversion is carried out by using a mixture containing an enantioselective acylating enzyme, which enzyme mixture is prepared by mixing an aqueous solution of the enantioselective acylating enzyme with an organic compound which forms an azeotrope with water and by subsequently azeotropically removing the water.

RX(2) OF 9 **A** + G ===> **H**



A G H YIELD 87%

RX(2) RCT A **98-86-2**

STAGE(1)
RGT C 67-63-0 Me2CHOH
CAT 19196-63-5 Benzeneacetamide, α-amino-α-methyl-, 584-08-7 K2CO3, **52462-29-0** Ruthenium, di-μ-chlorodichlorobis[(1,2,3,4,5,6-η)-1-methyl-4-(1-methylethyl)benzene]di-
CON 1 hour, 70 deg C

STAGE(2)
RCT G 108-22-5
CAT 9001-62-1 Lipase, 584-08-7 K2CO3
SOL 108-88-3 PhMe
CON 24 hours, 70 deg C

PRO H **16197-92-5**
NTE biotransformation, **enzymic**(Novozym 525L used second stage), **stereoselective**(second stage), alternate preparations also described, K2CO3/**enzyme** batch can be recovered and reused at least four times

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L133 ANSWER 5 OF 42 CASREACT COPYRIGHT 2007 ACS on STN

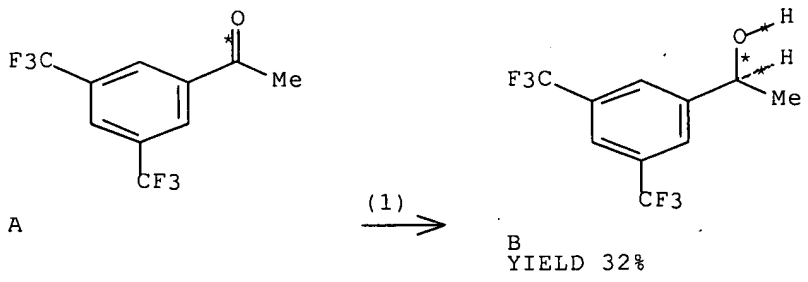
ACCESSION NUMBER: 143:365756 CASREACT Full-text
TITLE: Chemoenzymic synthesis of chiral secondary alcohols
INVENTOR(S): Dax, Thomas; Stanek, Michael; Poechlauer, Peter
PATENT ASSIGNEE(S): DSM Fine Chemicals Austria Nfg GmbH & Co Kg, Austria
SOURCE: PCT Int. Appl., 21 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005095628	A1	20051013	WO 2005-EP1977	20050225
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AT 500556	A1	20060115	AT 2004-471	20040318
EP 1725674	A1	20061129	EP 2005-707624	20050225
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR				
PRIORITY APPLN. INFO.:			AT 2004-471	20040318
			WO 2005-EP1977	20050225

OTHER SOURCE(S): MARPAT 143:365756

AB Disclosed is a chemoenzymic method for producing chiral secondary alcs. from ketones. The process consists of a chemical reduction of the ketone to a racemic alc. followed by a lipase catalyzed transesterification of the R-enantiomer. The unreacted S-alc. is then recovered by distillation. The remaining R-ester can then be hydrolyzed and the R-alc may be recycled back into the reaction mixture

RX(1) OF 1 **A** ===> **B**



A

B
YIELD 32%

RX(1) RCT A 30071-93-3

STAGE(1)
RGT C 19196-63-5 Benzeneacetamide, α-amino-α-methyl-, D 584-08-7 K2CO3
CAT **52462-29-0** Ruthenium, di-μ-chlorodichlorobis[(1,2,3,4,5,6-η)-1-methyl-4-(1-methylethyl)benzene]di-
SOL 67-63-0 Me2CHOH
CON 1 hour, 85 deg C

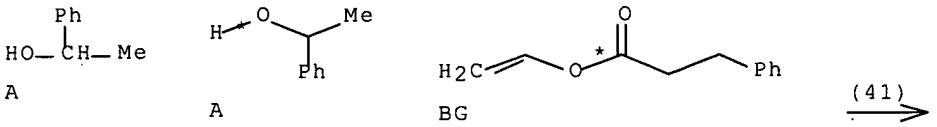
STAGE(2)
CAT 9001-62-1 Lipase
SOL 105-38-4 Propanoic acid, ethenyl ester
CON 4 hours, 70 deg C, 300 mbar

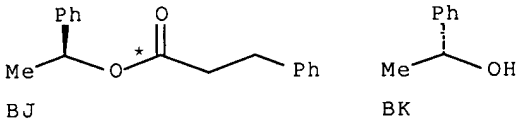
PRO B **225920-05-8**
NTE **stereoselective**, Novozyme435 used in stage 2, second stage biotransformation, second stage **enzymic**

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L133 ANSWER 6 OF 42 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 143:381652 CASREACT Full-text
TITLE: How Substrate Solvation Contributes to the Enantioselectivity of Subtilisin toward Secondary Alcohols
AUTHOR(S): Savile, Christopher K.; Kazlauskas, Romas J.
CORPORATE SOURCE: Department of Chemistry, McGill University, Montreal, QC, H3A 2K6, Can.
SOURCE: Journal of the American Chemical Society (2005), 127(35), 12228-12229
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The current rule to predict the enantiopreference of subtilisin toward secondary alcs. is based on the size of the substituents at the stereocenter and implies that the active site contains two differently sized pockets for these substituents. Several expts. are inconsistent with the current rule. First, the X-ray structures of subtilisin show there is only one pocket (the S1' pocket) approx. the size of a Ph group to bind secondary alcs. Second, the rule often predicts the incorrect enantiomer for reactions in water. To resolve these contradictions, we refine the current rule to show that subtilisin binds only one substituent of a secondary alc. and leaves the other in solvent. To test this refined empirical rule, we show that the enantioselectivity of a series of secondary alcs. in water varied linearly with the difference in hydrophobicity (log P/PO) of the substituents. This hydrophobicity difference accounts for the solvation of one substituent in water.

RX(41) OF 151 ...2 **A** + BG ===> BJ + **BK**



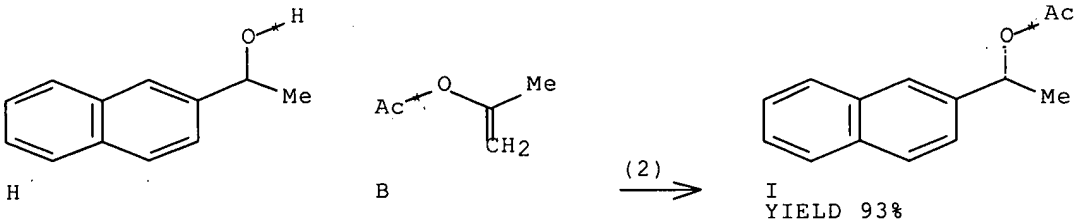


RX(41) RCT A 98-85-1, BG 54519-07-2
PRO BJ 52126-27-9, BK 1517-69-7
CAT 9014-01-1 Subtilisin
SOL 123-91-1 Dioxane
CON >48 hours, 30 deg C
NTE biotransformation, enzymic(recombinant subtilisin BPN' expressed in protease deficient Bacillus subtilis DB104 used), stereoselective(depends on enzyme and solvent), solid-supported catalyst(KCl)
REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L133 ANSWER 7 OF 42 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 143:152899 CASREACT Full-text
TITLE: Combined Ruthenium(II) and Lipase Catalysis for Efficient Dynamic Kinetic Resolution of Secondary Alcohols. Insight into the Racemization Mechanism
AUTHOR(S): Martin-Matute, Belen; Edin, Michaela; Bogar, Krisztian; Kaynak, F. Betuel; Baeckvall, Jan-E.
CORPORATE SOURCE: Department of Organic Chemistry, Arrhenius Laboratory, Stockholm University, Stockholm, SE-106 91, Swed.
SOURCE: Journal of the American Chemical Society (2005), 127(24), 8817-8825
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Pentaphenylcyclopentadienyl ruthenium complexes (3) are excellent catalysts for the racemization of secondary alcs. at ambient temperature The combination of this process with enzymic resolution of the alcs. results in a highly efficient synthesis of enantiomerically pure acetates at room temperature with short reaction times for most substrates. This new reaction was applied to a wide range of functionalized alcs. including heteroarom. alcs., and for many of the latter, enantiopure acetates were efficiently prepared for the first time via dynamic kinetic resolution (DKR). Different substituted cyclopentadienyl ruthenium complexes were prepared and studied as catalysts for racemization of alcs. Pentaaryl-substituted cyclopentadienyl complexes were found to be highly efficient catalysts for the racemization. Substitution of one of the aryl groups by an alkyl group considerably slows down the racemization process. A study of the racemization of (S)-1-phenylethanol catalyzed by ruthenium hydride η5-Ph5CpRu(CO)2H (8) indicates

that the racemization takes place within the coordination sphere of the ruthenium catalyst. This conclusion was supported by the lack of ketone exchange in the racemization of (S)-1-phenylethanol performed in the presence of p-tolyl Me ketone (1 equiv), which gave <1% of 1-(p-tolyl)ethanol. The structures of ruthenium chloride and iodide complexes 3a and 3c and of ruthenium hydride complex 8 were confirmed by X-ray anal.

RX(2) OF 68 H + B ===> I



RX(2)

STAGE(1)
RGT D 865-47-4 t-BuOK, E 497-19-8 Na2CO3
CAT **677736-23-1** Ruthenium, dicarbonylchloro[(1,2,3,4,5-η)-1,2,3,4,5-pentaphenyl-2,4-cyclopentadien-1-yl]-
SOL 108-88-3 PhMe
CON 6 minutes, room temperature

STAGE(2)
RCT H **7228-47-9**
CON 4 minutes, room temperature

STAGE(3)
RCT B 108-22-5
CON 3 hours, room temperature

PRO I **84194-78-5**
NTE biotransformation, **enzymic**, Candida antarctica lipse B used in stage 1, **stereoselective**

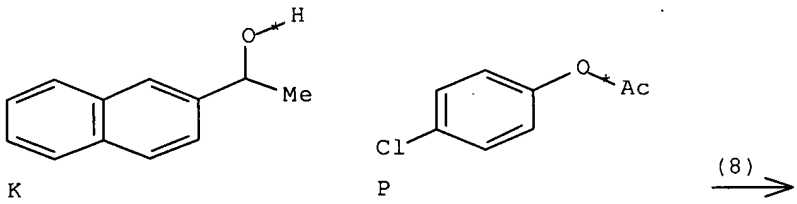
REFERENCE COUNT: 116 THERE ARE 116 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L133 ANSWER 8 OF 42 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 143:43627 CASREACT Full-text
TITLE: Dynamic kinetic resolution of secondary alcohols with a readily available ruthenium-based racemization catalyst
AUTHOR(S): Riermeier, Thomas H.; Gross, Peter; Monsees, Axel; Hoff, Manfred; Trauthwein, Harald
CORPORATE SOURCE: Degussa AG, Degussa Homogeneous Catalysts, Hanau-Wolfgang, D-63457, Germany

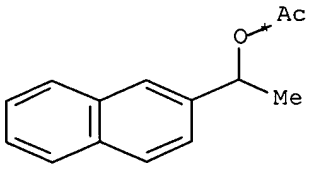
SOURCE: Tetrahedron Letters (2005), 46(19), 3403-3406
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB An easy to handle and stable racemization catalyst for secondary alcs. is obtained by an in situ mixture of readily available [Ru(cymene)Cl2]2 with chelating aliphatic diamines. Optimization of the reaction revealed that N,N,N',N'-tetramethyl-1,3-propanediamine as ligand racemizes aromatic alcs. completely within 5 h. This easy to handle and stable catalytic system is combined with a lipase-catalyzed resolution to provide an efficient dynamic kinetic resolution of secondary alcs.

RX(8) OF 14 ...K + P ===> T



K P



T
YIELD 64%

RX(8)

STAGE(1)
CAT 52462-29-0 Ruthenium, di-μ-chlorodichlorobis[(1,2,3,4,5,6-η)-1-methyl-4-(1-methylethyl)benzene]di-, 110-95-2 1,3-Propanediamine, N,N,N',N'-tetramethyl-
SOL 108-88-3 PhMe
CON 10 minutes, room temperature

STAGE(2)
RCT K 7228-47-9, P 876-27-7
RGT U 93-08-3 Ethanone, 1-(2-naphthalenyl)-
CAT 9001-62-1 Lipase
CON 45 hours, 80 deg C

PRO T 32860-25-6
NTE biotransformation, stereoselective, enzymic

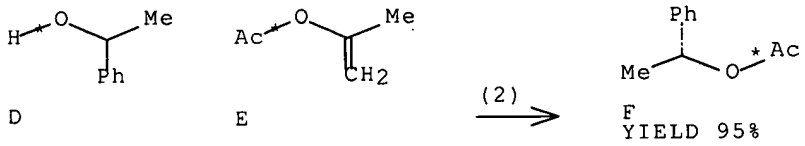
(Candida antarctica B lipase used), dynamic kinetic resolution allows for greater than 50% conversion and yield, lower yield if ketone omitted second stage

REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L133 ANSWER 9 OF 42 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 143:76919 CASREACT Full-text
TITLE: Removal of the acyl donor residue allows the use of simple alkyl esters as acyl donors for the dynamic kinetic resolution of secondary alcohols
AUTHOR(S): Verzijl, Gerard K. M.; de Vries, Johannes G.; Broxterman, Quirinus B.
CORPORATE SOURCE: Life Sciences-Advanced Synthesis, Catalysis and Development, DSM Research, Geleen, 6160 MD, Neth.
SOURCE: Tetrahedron: Asymmetry (2005), 16(9), 1603-1610
CODEN: TASYE3; ISSN: 0957-4166
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The dynamic kinetic resolution of secondary alcs. using a lipase and a ruthenium catalyst as developed by Baeckvall required some improvements to make it suitable for its use in an industrial process. The use of p-chlorophenyl acetate as acyl donor is not desirable in view of the toxicity of the side product. We herein report that simple alkyl esters can be used as acyl donors if the alc. or ketone residue formed during the enzymic acylation is continuously removed during the reaction. The addition of a ketone speeds up the racemization process and allowed us to reduce the amts. of enzyme and ruthenium catalyst. The scope of this method was explored and a suitable range of acyl donors found. Various benzylic and aliphatic alcs. were reacted using iso-Pr butyrate or Me phenylacetate as acyl donor and in most cases the ester was isolated in >95% yield and 99% ee. Furthermore, it was demonstrated that the alc. byproducts of the enzymic resolution could be used as the hydrogen source in the asym. reductive transesterification of ketones.

RX(2) OF 20 D + E ===> F



D E F
YIELD 95%

RX(2) RCT D **98-85-1**, E 108-22-5
PRO F **16197-92-5**
CAT 9001-62-1 Lipase, 98-86-2 Acetophenone, **104439-77-2** Ruthenium, tetracarbonyl-μ-hydro[(1,2,3,4,5-η)-1-hydroxylato-2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl][(1,2,3,4,5-η)-1-hydroxy-2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl]di-
SOL 108-88-3 PhMe
CON 24 hours, 70 deg C, 215 mbar

NTE biotransformation, **enzymic, stereoselective,** optimization study(optimized on catalyst ratios, pressure), alternate preparations also described

REFERENCE COUNT: 49 THERE ARE 49 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L133 ANSWER 10 OF 42 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 144:253689 CASREACT Full-text

TITLE: (S)-selective kinetic resolution and chemoenzymatic dynamic kinetic resolution of secondary alcohols

AUTHOR(S): Boren, Linnea; Martin-Matute, Belen; Xu, Yongmei; Cordova, Armando; Baeckvall, Jan-E.

CORPORATE SOURCE: Department of Organic Chemistry, Arrhenius Laboratory, Stockholm University, Stockholm, 106 91, Swed.

SOURCE: Chemistry--A European Journal (2005), Volume Date 2006, 12(1), 225-232
CODEN: CEUJED; ISSN: 0947-6539

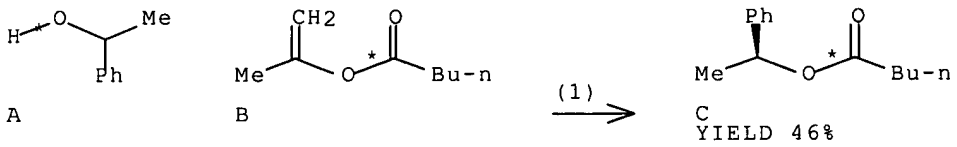
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA

DOCUMENT TYPE: Journal

LANGUAGE: English

AB (S)-Selective kinetic resolution was achieved through the use of a com. available protease, which was activated with a combination of two different surfactants. The kinetic resolution (KR) process was optimized with respect to activation of the protease and to the acyl donor. The KR proved to be compatible with a range of functionalized sec-alcs., giving good to high enantiomeric ratio values (up to >200). The enzymic resolution was combined with a ruthenium-catalyzed racemization to give an (S)-selective dynamic kinetic resolution (DKR) of sec-alcs. The DKR process works under very mild reaction conditions to give the corresponding esters in high yields and with excellent enantioselectivities.

RX(1) OF 17 **A** + B ===> **C**



A B C
YIELD 46%

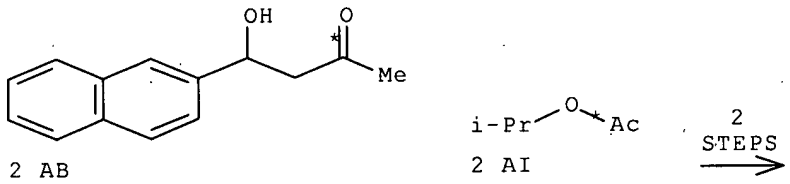
RX(1) RCT A **98-85-1**, B 69638-96-6
RGT D 497-19-8 Na2CO3
PRO C **183184-17-0**
CAT **9014-01-1** Subtilisin, 29836-26-8 β-D-Glucopyranoside, octyl, 9004-95-9 Poly(oxy-1,2-ethanediyl), α-hexadecyl-ω-hydroxy-
SOL 109-99-9 THF
CON 17 hours, room temperature
NTE biotransformation, enzymic, stereoselective, yield depends on catalyst activator

REFERENCE COUNT: 55 THERE ARE 55 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

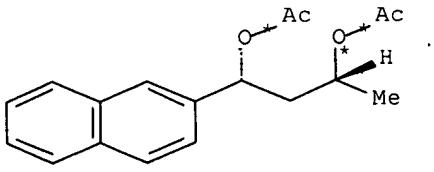
L133 ANSWER 11 OF 42 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 141:71330 CASREACT Full-text
TITLE: One-pot synthesis of enantiopure syn-1,3-diacetates from racemic syn/anti mixtures of 1,3-diols by dynamic kinetic asymmetric transformation
AUTHOR(S): Edin, Michaela; Steinreiber, Johannes; Baeckvall, Jan-E.
CORPORATE SOURCE: Department of Organic Chemistry, Arrhenius Laboratory, Stockholm University, Stockholm, SE-106 91, Swed.
SOURCE: Proceedings of the National Academy of Sciences of the United States of America (2004), 101(16), 5761-5766
CODEN: PNASA6; ISSN: 0027-8424
PUBLISHER: National Academy of Sciences
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A one-pot synthesis of enantiomerically pure syn-1,3-diacetates starting from readily accessible racemic diastereomeric mixts. of 1,3-diols has been realized by combining (i) enzymic transesterification, (ii) ruthenium-catalyzed epimerization of a secondary alc. in a diol or diol monoacetate, and (iii) intramol. acyl migration in a syn-1,3-diol monoacetate. The in situ coupling of these three processes results in an efficient enantioselective synthesis of acyclic syn-1,3-diacetates via combined deracemization-deepimerization and constitutes a dynamic kinetic asym. transformation concept. Several differently substituted unsym., acyclic syn-1,3-diacetates were obtained in yields up to 73% with excellent enantioselectivities (>99%) and good diastereomeric ratios (>90% syn).

RX(33) OF 34 COMPOSED OF RX(23), RX(20)
RX(33) 2 **AB** + 2 AI ===> **AM**



2 AB
2 AI



AM
YIELD 53%

RX(23) RCT AB **229156-79-0**

STAGE(1)
RGT P 16940-66-2 NaBH4
SOL 67-56-1 MeOH
CON 1 hour, room temperature

STAGE(2)
SOL 7732-18-5 Water
CON room temperature

PRO AL 712342-54-6, AP 712342-65-9
NTE **stereoselective**

RX(20) RCT AL 712342-54-6, AI 108-21-4

STAGE(1)
CAT **104439-77-2** Ruthenium, tetracarbonyl-μ-hydro[(1,2,3,4,5-η)-1-hydroxylato-2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl][(1,2,3,4,5-η)-1-hydroxy-2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl]di-, 9001-62-1 Lipase
SOL 108-88-3 PhMe
CON SUBSTAGE(1) 12 hours, 70 deg C
SUBSTAGE(2) 70 deg C -> room temperature

STAGE(2)
RGT J 1333-74-0 H2
CON SUBSTAGE(1) 12 hours, room temperature
SUBSTAGE(2) 45 hours, 70 deg C

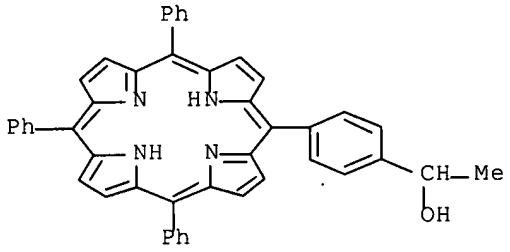
PRO AM **712342-62-6**
NTE biotransformation, **enzymic**

REFERENCE COUNT: 55 THERE ARE 55 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

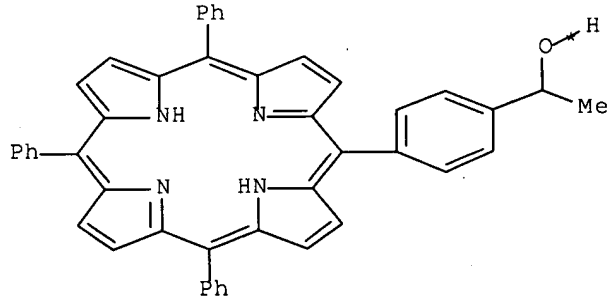
L133 ANSWER 12 OF 42 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 136:365670 CASREACT Full-text
TITLE: 5-[4-(1-Hydroxyethyl)phenyl]-10,15,20-triphenylporphyrin as a Probe of the Transition-State Conformation in Hydrolase-Catalyzed Enantioselective Transesterifications
AUTHOR(S): Ema, Tadashi; Jittani, Masahito; Furuie, Kenji; Utaka, Masanori; Sakai, Takashi
CORPORATE SOURCE: Department of Applied Chemistry, Faculty of Engineering, Okayama University, Tsushima, Okayama, 700-8530, Japan
SOURCE: Journal of Organic Chemistry (2002), 67(7), 2144-2151
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB 5-[4-(1-Hydroxyethyl)phenyl]-10,15,20-triphenylporphyrin (1a) and zinc porphyrin 1b were designed and synthesized to exptl. examine the validity of the transition-state model previously proposed for the lipase-catalyzed kinetic resolution of secondary alcs. The lipases from Pseudomonas cepacia (lipase PS), Candida antarctica (CHIRAZYME L-2), Rhizomucor miehei (CHIRAZYME L-9), and Pseudomonas aeruginosa (lipase LIP) exhibited excellent enantioselectivity (E >100 at 30°). Subtilisin Carlsberg from Bacillus licheniformis (ChiroCLEC-BL) also showed high enantioselectivity for 1a (E =

140 at 30°), and the thermodn. parameters were determined: ΔΔH.dbldag. = -6.8±0.8 kcal mol-1, ΔΔS.dbldag. = -13±3 cal mol-1 K-1. Lipases and subtilisin showed R- and S-preference for 1, resp. The mechanisms underlying the exptl. observations are explained in terms of the transition-state models. The large secondary alc. 1 is a powerful tool for investigating the conformation of the transition state of the enzyme-catalyzed reactions. The fact that 1 was resolved with high enantioselectivity strongly suggests that the gauche conformation, but not the anti conformation, is taken in the transition state, in agreement with the transition-state models involving the stereoelectronic effect.

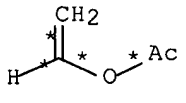
RX(3) OF 10 ...2 **D** + L ===> **M** + N



D

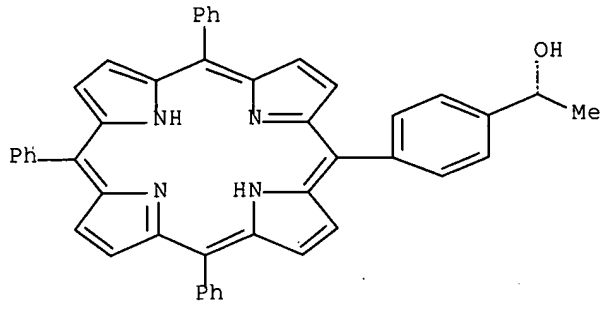


D

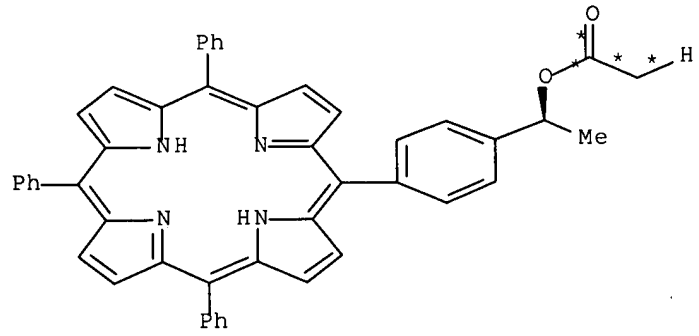


L

(3) →



M



N

RX(3) RCT D **153721-59-6**, L 108-05-4
PRO M **239080-08-1**, N 422510-55-2
CAT **9014-01-1** Subtilisin
SOL 108-20-3 Isopropyl ether
NTE enzymic, stereoselective, optimization study, optimized on time,temp, resoln. step, sepn. by column chromatog. on silica gel

REFERENCE COUNT: 56 THERE ARE 56 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L133 ANSWER 13 OF 42 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 136:4770 CASREACT Full-text
TITLE: Process for the preparation of enantiomerically enriched esters and alcohols
INVENTOR(S): Verzijl, Gerardus Karel Maria; De Vries, Johannes Gerardus; Broxterman, Quirinus Bernardus
PATENT ASSIGNEE(S): DSM N.V., Neth.
SOURCE: PCT Int. Appl., 43 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

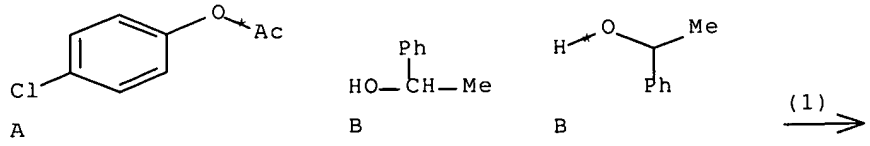
WO 2001090396	A1	20011129	WO 2001-NL383	20010521
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
NL 1015313	C2	20011127	NL 2000-1015313	20000526
CA 2410529	A1	20011129	CA 2001-2410529	20010521
EP 1283898	A1	20030219	EP 2001-932412	20010521
EP 1283898	B1	20060510		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
HU 200302361	A2	20031028	HU 2003-2361	20010521
JP 2003533993	T	20031118	JP 2001-586591	20010521
AT 325888	T	20060615	AT 2001-932412	20010521
IN 2002CN01933	A	20050211	IN 2002-CN1933	20021125
US 2004077059	A1	20040422	US 2002-296840	20021126
US 6841691	B2	20050111		
PRIORITY APPLN. INFO.:			NL 2000-1015313	20000526
			WO 2001-NL383	20010521

got it

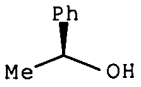
OTHER SOURCE(S): MARPAT 136:4770

AB Method for the preparation of an enantiomerically enriched ester, in which a mixture of the enantiomers of the corresponding secondary alc. is subjected, in the presence of an acyl donor, to an enantioselective conversion in the presence of a racemization catalyst upon which the ester is formed and an acyl donor residue is obtained, and in which the acyl donor residue is irreversibly removed from the phase in which the enantioselective conversion takes place. Preferably the enantioselective conversion is carried out enzymically and a transfer hydrogenation catalyst is used as racemization catalyst. The secondary alc. can be formed in situ from the corresponding ketone, in the presence of a H donor. It is also possible to use a mixture of the secondary alc. and the corresponding ketone as substrate. Preferably the acyl donor is chosen so that the acyl donor residue is converted in situ into another compound and/or the acyl donor residue is removed via distillation under reduced pressure. The enantiomerically enriched esters obtained can subsequently be converted into the corresponding enantiomerically enriched alcs., which are desirable intermediate products in the preparation of liquid crystals, agro chems. or pharmaceuticals.

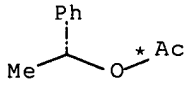
RX(1) OF 8 A + 2 B ===> C + D



A B B



C
YIELD 32%



D
YIELD 62%

RX(1) RCT A 876-27-7, B **98-85-1**
PRO C **1445-91-6**, D 16197-92-5
CAT 9001-62-1 Lipase, **104439-77-2** Ruthenium, tetracarbonyl-μ-hydro[(1,2,3,4,5-η)-1-hydroxylato-2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl][(1,2,3,4,5-η)-1-hydroxy-2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl]di-
SOL 108-88-3 PhMe
NTE **stereoselective, enzymic**, biotransformation, alternative prepn.gave lower yields and various selectivity for the alc.

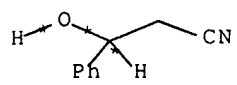
REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L133 ANSWER 14 OF 42 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 136:37080 CASREACT Full-text
TITLE: Efficient lipase-catalyzed kinetic resolution and dynamic kinetic resolution of β-hydroxy nitriles. A route to useful precursors for γ-amino alcohols
AUTHOR(S): Pamies, Oscar; Backvall, Jan-E.
CORPORATE SOURCE: Department of Organic Chemistry, Arrhenius Laboratory, Stockholm University, Stockholm, 106 91, Swed.
SOURCE: Advanced Synthesis & Catalysis (2001), 343(6+7), 726-731
CODEN: ASCAF7; ISSN: 1615-4150
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English

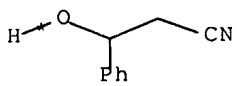
qpt

AB An efficient kinetic resolution of racemic β-hydroxy nitriles was performed via Candida antarctica lipase (N-435)-catalyzed transesterification. A variety of racemic alkyl, aryl, and aryloxymethyl substituted β-hydroxy nitriles was efficiently transformed to the corresponding enantiomerically pure acetates (ee >99% and conversion = 50%) with E values from 40 to >1000. The combination of the enzymic kinetic resolution with a ruthenium-catalyzed alc. racemization led to a dynamic kinetic resolution (ee's up to 99%, yields up to 85%).

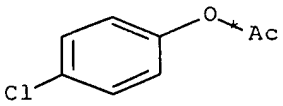
RX(13) OF 67 ...2 **C** + AF ===> **AG** + AJ



C

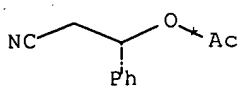


C

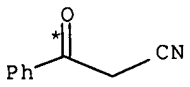


AF

(13) →



AG
YIELD 74%



AJ
YIELD 23%

RX(13) RCT C **17190-29-3**, AF 876-27-7
PRO AG **21087-76-3**, AJ 614-16-4
CAT **104439-77-2** Ruthenium, tetracarbonyl-μ-hydro[(1,2,3,4,5-η)-1-hydroxylato-2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl][(1,2,3,4,5-η)-1-hydroxy-2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl]di-, 9001-62-1 Lipase
SOL 108-88-3 PhMe
NTE **stereoselective, enzymic**, candida antarctica B (N-435) lipase used, biotransformation, regioselective

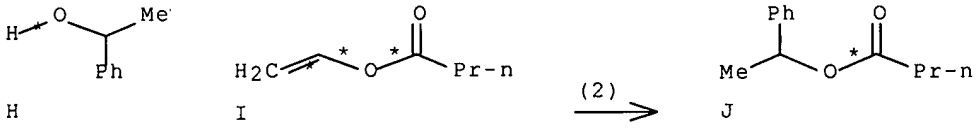
REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L133 ANSWER 15 OF 42 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 135:238582 CASREACT Full-text
TITLE: Effect of crown ethers on structure, stability, activity, and enantioselectivity of subtilisin carlsberg in organic solvents
AUTHOR(S): Santos, Angelica M.; Vidal, Michael; Pacheco, Yamaris; Frontera, Joel; Baez, Carlos; Ornellas, Olivia; Barletta, Gabriel; Griebenow, Kai
CORPORATE SOURCE: Department of Chemistry, University of Puerto Rico, San Juan, 00931-3346, P. R.
SOURCE: Biotechnology and Bioengineering (2001), 74(4), 295-308
CODEN: BIBIAU; ISSN: 0006-3592
PUBLISHER: John Wiley & Sons, Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English

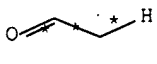
AB Co-lyophilization or co-drying of subtilisin Carlsberg with the crown ethers 18-crown-6, 15-crown-5, and 12-crown-4 substantially improved enzyme activity in THF, acetonitrile, and 1,4-dioxane in the transesterification reactions of N-acetyl-L-phenylalanine Et ester and 1-propanol and that of (±)-1-phenylethanol and vinyl butyrate. The acceleration of the initial rate, Vo, ranged from less than 10-fold to more than 100-fold. All crown ethers activated subtilisin substantially, which excludes a specific macrocyclic effect from being responsible. The secondary structure of subtilisin was studied by Fourier-transform IR (FTIR) spectroscopy. 18-Crown-6 and 15-crown-5 led to a more native-like structure of subtilisin in the organic solvents employed when compared with that of the dehydrated enzyme obtained from buffer alone. However, the high level of activation with 12-crown-4 where this effect was not observed excluded overall structural preservation from being the primary cause of the observed enzyme activation. The conformational mobility of subtilisin was investigated by performing thermal denaturation expts. in 1,4-dioxane. Although only a small effect of temperature on subtilisin structure was observed for the samples prepared with or without 12-crown-4, both 18-crown-6 and 15-crown-5 caused the enzyme to denature at quite

low temps. (38° and 56°, resp.). No relationship between this property and Vo was evident, but increased conformational mobility of the protein decreased its storage stability. The possibility of a "mol. imprinting" effect was also tested by removing 18-crown-6 from the subtilisin-18-crown-6 co-lyophilizate by washing. Vo was only halved as a result of this procedure, an effect insignificant compared with the ca. 80-fold rate enhancement observed prior to washing in THF. This suggests that mol. imprinting is likely the primary cause of subtilisin activation by crown ethers, as recently suggested.

RX(2) OF 2 **H** + I ===> **J** + K



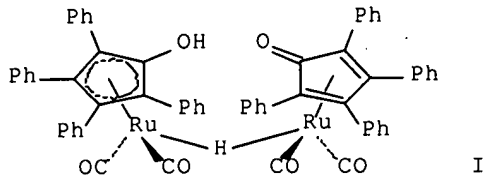
H I J



K

RX(2) RCT H **98-85-1**, I 123-20-6
RGT E 294-93-9 12-Crown-4
PRO J **3460-44-4**, K 75-07-0
CAT **9014-01-1** Subtilisin
SOL 109-99-9 THF
NTE biotransformation, enzymic, optimization study
REFERENCE COUNT: 58 THERE ARE 58 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

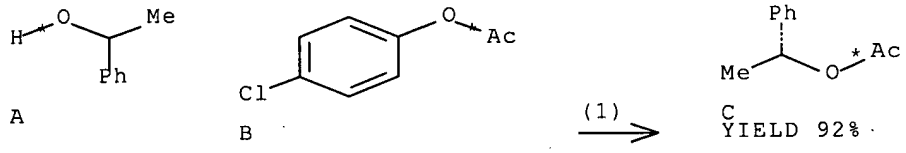
L133 ANSWER 16 OF 42 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 127:135610 CASREACT Full-text
TITLE: Enzymic resolution of alcohols coupled with ruthenium-catalyzed racemization of the substrate alcohol
AUTHOR(S): Larsson, Anna L. E.; Persson, B. Anders; Backvall, Jan-E.
CORPORATE SOURCE: Department Organic Chemistry, Uppsala University, Uppsala, S-75121, Swed.
SOURCE: Angewandte Chemie, International Edition in English (1997), 36(11), 1211-1212
CODEN: ACIEAY; ISSN: 0570-0833
PUBLISHER: Wiley-VCH
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

AB The ruthenium-catalyzed racemization of (+)-(R)-α- methylbenzenemethanol was coupled with an enzyme-catalyzed transesterification to give the resolved alc. derivative Thus, the combination of catalyst I, 4-chlorophenyl acetate and Novozym 435 in the reaction of (+)-(R)-α-methylbenzenemethanol gave (R)-α-methylbenzenemethanol acetate in high yield and high enantiomeric purity.

RX(1) OF 2 **A** + B ===> **C**



A B C YIELD 92%

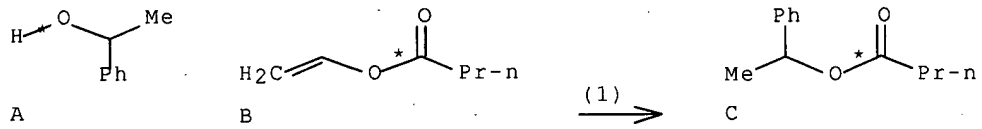
RX(1) RCT A **98-85-1**, B 876-27-7
RGT D 9001-62-1 Lipase
PRO C **16197-92-5**
CAT **104439-77-2** Ruthenium, tetracarbonyl-μ-hydro[(1,2,3,4,5-η)-1-hydroxylato-2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl][(1,2,3,4,5-η)-1-hydroxy-2,3,4,5-tetraphenyl-2,4-cyclopentadien-1-yl]di-
SOL 75-65-0 t-BuOH
NTE acetophenone also present, biotransformation, **enzymic, stereoselective**, other acetate sources gave lower conversions with equal selectivity

REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L133 ANSWER 17 OF 42 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 114:159632 CASREACT Full-text
TITLE: How can the solvent affect enzyme enantioselectivity?
AUTHOR(S): Fitzpatrick, Paul A.; Klibanov, Alexander M.
CORPORATE SOURCE: Dep. Chem., Massachusetts Inst. Technol., Cambridge, MA, 02139, USA
SOURCE: Journal of the American Chemical Society (1991), 113(8), 3166-71
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The enantioselectivity of subtilisin Carlsberg in the transesterification between the chiral alc., sec-phenethyl alc., and vinyl butyrate was found to

be greatly affected by the solvent; e.g., the (kcat/km)S/(kcat/Km)R ratio varied from 3 in anhydrous acetonitrile of 61 in anhydrous dioxane. A mechanistic model was proposed that explained these findings. This model was supported by exptl. data obtained concerning the dependence of subtilisin's enantioselectivity on the structure of the chiral alc., on physicochem. characteristics of the solvent (systematic correlations were found with the dielec. constant and dipole moment), and on such additives as water and the water mimic, formamide. Similar dependencies (although of a smaller magnitude) were observed for the related enzyme, subtilisin BPN'.

RX(1) OF 1 **A** + **B** ===> **C**



RX(1) RCT A **98-85-1**, B 123-20-6
PRO C **3460-44-4**
CAT **9014-01-1** Subtilisin
NTE Biotransformation: catalyzed by subtilisin

L133 ANSWER 18 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:453821 CAPLUS Full-text
DOCUMENT NUMBER: 145:62617
TITLE: Asymmetric transfer hydrogenation of α,β-unsaturated, α-tosyloxy and α-substituted ketones. [Erratum to document cited in CA144:369714]
AUTHOR(S): Hannedouche, Jerome; Peach, Philip; Cross, David J.; Kenny, Jennifer A.; Mann, Inderjit; Houson, Ian; Campbell, Lynne; Walsgrove, Tim; Wills, Martin
CORPORATE SOURCE: Department of Chemistry, University of Warwick, Coventry, CV4 7AL, UK
SOURCE: Tetrahedron (2006), 62(23), 5549
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 16 May 2006
AB On page 1864, the author line is incorrect; the third author Jerome Hannedouche was omitted.
CC 25-7 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
IT **Alcohols, preparation**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(allyl; preparation of α,β-unsatd. ketones and their chemoselective, stereoselective, and enantioselective reduction to allylic alcs. by transfer hydrogenation in the presence of nonracemic rhodium

and ruthenium diamine complexes (Erratum))
IT **Resolution (separation)**
(**kinetic, dynamic**; stereoselective and enantioselective preparation of alcs. by transfer hydrogenation and **dynamic kinetic** resolution of ketones in the presence of nonracemic rhodium and ruthenium diamine complexes (Erratum))
IT **Alcohols, preparation**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(stereoselective and enantioselective preparation of alcs. and allylic alcs.
by transfer hydrogenation of ketones, α,β-enones, and α-tosyloxy ketones in the presence of nonracemic rhodium and ruthenium diamine complexes (Erratum))
IT 12354-85-7, Bis(pentamethylcyclopentadienylrhodium dichloride) **52462-29-0**, (p-Cymene)ruthenium(II) chloride dimer 144222-34-4, N-[(1R,2R)-2-Amino-1,2-diphenylethyl]-4-methylbenzenesulfonamide 167316-27-0, (1S,2S)-(+)-N-p-Tosyl-1,2-diphenylethylenediamine **882022-88-0**
RL: **CAT (Catalyst use)**; USES (Uses)
(stereoselective and enantioselective preparation of alcs. and allylic alcs.
by transfer hydrogenation of ketones, α,β-enones, and α-tosyloxy ketones in the presence of nonracemic rhodium and ruthenium diamine complexes (Erratum))

L133 ANSWER 19 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:124021 CAPLUS Full-text
DOCUMENT NUMBER: 144:369675
TITLE: Resolution of Racemic 2-Aminocyclohexanol Derivatives and Their Application as Ligands in Asymmetric Catalysis
AUTHOR(S): Schiffers, Ingo; Rantanen, Toni; Schmidt, Frank; Bergmans, Werner; Zani, Lorenzo; Bolm, Carsten
CORPORATE SOURCE: Institut fuer Organische Chemie, RWTH Aachen, Aachen, D-52056, Germany
SOURCE: Journal of Organic Chemistry (2006), 71(6), 2320-2331
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 144:369675
ED Entered STN: 10 Feb 2006
AB A preparatively easy and efficient protocol for the resolution of racemic 2-aminocyclohexanol derivs. is described, delivering both enantiomers with >99% enantiomeric excess (ee) by sequential use of (R)- and (S)-mandelic acid. A simple aqueous workup procedure permits the isolation of the amino alcs. in anal. pure form and the almost quant. recovery of mandelic acid. Debenzylation of enantiopure trans-2-(benzylamino)-1-cyclohexanol by hydrogenation and subsequent derivatization give access to a broad variety of diversely substituted derivs. Furthermore, the corresponding cis isomers are readily available. Applications of these optically active aminocyclohexanols in catalyzed asym. Ph transfer reactions to benzaldehydes and transfer hydrogenations of aryl ketones lead to products with up to 96% ee.
CC 24-5 (Alicyclic Compounds)
IT **Ketones, reactions**
RL: RCT (Reactant); RACT (Reactant or reagent)
(alkyl aromatic; preparation of enantiopure 2-aminocyclohexanols and analogs

via resolution of **racemic** derivs. with mandelic acids and their use as chiral ligands in asym. Ph transfer reaction to benzaldehydes and transfer hydrogenation of aryl ketones)

IT **Alcohols, preparation**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(benzyl; preparation of enantiopure 2-aminocyclohexanols and analogs via resolution of racemic derivs. with mandelic acids and their use as chiral ligands in asym. Ph transfer reaction to benzaldehydes and transfer hydrogenation of aryl ketones)

IT **Alcohols, preparation**
RL: CAT (Catalyst use); SPN (Synthetic preparation); **PREP (Preparation)**; USES (Uses)
(chiral, amino; preparation of enantiopure 2-aminocyclohexanols and analogs via resolution of racemic derivs. with mandelic acids and their use as chiral ligands in asym. Ph transfer reaction to benzaldehydes and transfer hydrogenation of aryl ketones)

IT Arylation catalysts
Asymmetric synthesis and induction
Resolution (separation)
(preparation of enantiopure 2-aminocyclohexanols and analogs via resolution of racemic derivs. with mandelic acids and their use as chiral ligands in asym. Ph transfer reaction to benzaldehydes and transfer hydrogenation of aryl ketones)

REFERENCE COUNT: 217 THERE ARE 217 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L133 ANSWER 20 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:115656 CAPLUS Full-text
DOCUMENT NUMBER: 144:369714
TITLE: Asymmetric transfer hydrogenation of α,β-unsaturated, α-tosyloxy and α-substituted ketones
AUTHOR(S): Peach, Philip; Cross, David J.; Kenny, Jennifer A.; Mann, Inderjit; Houson, Ian; Campbell, Lynne; Walsgrove, Tim; Wills, Martin
CORPORATE SOURCE: Department of Chemistry, University of Warwick, Coventry, CV4 7AL, UK
SOURCE: Tetrahedron (2006), 62(8), 1864-1876
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 144:369714
ED Entered STN: 08 Feb 2006
AB Asym. transfer hydrogenation of cyclic and acyclic α,β-unsatd. ketones catalyzed by ruthenium and rhodium diamine and amino alc. complexes have been investigated. Cyclic α,β-unsatd. ketones appeared to be more suitable substrates for the synthesis of enantiomerically pure allylic alcs. than do acyclic α,β-unsatd. ketones. A proposed mechanism for the formation of 4-phenyl[1,3]-2- dioxolanone from α-tosyloxy- and halo-substituted acetophenone derivs. is discussed. The results of further investigations into the reduction of a range of α-tosyloxyacetophenone derivs. and the dynamic kinetic resolution of α-substituted ketones is presented.
CC 25-7 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
IT **Alcohols, preparation**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)

(allyl; preparation of α,β-unsatd. ketones and their chemoselective, stereoselective, and enantioselective reduction to allylic alcs. by transfer hydrogenation in the presence of nonracemic rhodium and ruthenium diamine complexes)

IT **Resolution (separation)**
(**kinetic, dynamic**; stereoselective and enantioselective preparation of alcs. by transfer hydrogenation and **dynamic kinetic** resolution of ketones in the presence of nonracemic rhodium and ruthenium diamine complexes)

IT **Alcohols, preparation**
Ketones, preparation
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(stereoselective and enantioselective preparation of alcs. and allylic alcs.
by transfer hydrogenation of ketones, α,β-enones, and α-tosyloxy ketones in the presence of nonracemic rhodium and ruthenium diamine complexes)

IT 12354-85-7, Bis(pentamethylcyclopentadienylrhodium dichloride)
13472-33-8 **52462-29-0**, (p-Cymene)ruthenium(II) chloride dimer
126456-43-7 144222-34-4, N-[(1R,2R)-2-Amino-1,2-diphenylethyl]-4-methylbenzenesulfonamide 167316-27-0, (1S,2S)-(+)-N-p-Tosyl-1,2-diphenylethylenediamine **882022-88-0**
RL: **CAT (Catalyst use)**; USES (Uses)
(stereoselective and enantioselective preparation of alcs. and allylic alcs.
by transfer hydrogenation of ketones, α,β-enones, and α-tosyloxy ketones in the presence of nonracemic rhodium and ruthenium diamine complexes)

REFERENCE COUNT: 74 THERE ARE 74 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L133 ANSWER 21 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:220057 CAPLUS Full-text
DOCUMENT NUMBER: 145:292400
TITLE: Simple and recyclable oxidation, racemization and dynamic kinetic resolution of activated alcohols catalyzed by hydrated ruthenium chloride in aqueous medium
AUTHOR(S): Wolfson, Adi; Yehuda, Chen; Shokin, Olga; Tavor, Dorith
CORPORATE SOURCE: Chemical Engineering Department, Sami Shamoon College of Engineering, Beer Sheva, 84100, Israel
SOURCE: Letters in Organic Chemistry (2006), 3(2), 107-110
CODEN: LOCEC7; ISSN: 1570-1786
PUBLISHER: Bentham Science Publishers Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 13 Mar 2006
AB Employing water as medium for aerobic oxidation and dynamic kinetic resolution of activated alcs. with RuCl3, nH2O resulted in simple and recyclable catalytic systems.
CC 22-7 (Physical Organic Chemistry)
Section cross-reference(s): 7, 67
IT **Resolution (separation)**
(**kinetic, dynamic**; recyclable oxidation, racemization and **dynamic kinetic** resolution, DKR, of activated alcs. catalyzed by hydrated ruthenium chloride in aqueous medium)
IT **Alcohols, reactions**

RL: PNU (Preparation, unclassified); RCT (Reactant); **PREP (Preparation)**; RACT (Reactant or reagent)
(recyclable oxidation, racemization and dynamic kinetic resolution, DKR, of activated alcs. catalyzed by hydrated ruthenium chloride in aqueous medium)

IT **14898-67-0**
RL: **CAT (Catalyst use)**; USES (Uses)
(recyclable oxidation, racemization and dynamic kinetic resolution, DKR, of activated alcs. catalyzed by hydrated ruthenium chloride in aqueous medium)

REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L133 ANSWER 22 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:1116636 CAPLUS Full-text
DOCUMENT NUMBER: 143:440060
TITLE: Process for preparation of optically pure water-soluble 1,2-bis[2-(hydroxysulfonyl)phenyl]-1,2-ethylenediamine derivatives and application as asymmetric transfer hydrogenation catalysts
INVENTOR(S): Deng, Jingen; Ma, Yaping; Wang, Fei; Zhu, Jin; Cui, Xin
PATENT ASSIGNEE(S): Chengdu Institute of Organic Chemistry, Chinese Academy of Sciences, Peop. Rep. China
SOURCE: Faming Zhuanli Shenqing Gongkai Shuomingshu, 16 pp.
CODEN: CNXXEV
DOCUMENT TYPE: Patent
LANGUAGE: Chinese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CN 1566084	A	20050119	CN 2003-135181	20030612
PRIORITY APPLN. INFO.:			CN 2003-135181	20030612

OTHER SOURCE(S): CASREACT 143:440060
ED Entered STN: 18 Oct 2005
AB The invention relates to novel water-soluble diamine and its derivs., their preparation and application, specifically optically pure 1,2-bis[2-(hydroxysulfonyl)phenyl]-1,2-ethylenediamine derivs., their preparation and application in asym. catalysis. By using the ligand and transition metals (Group VIII) such as ruthenium, rhodium, and iridium as the asym. catalyst in aqueous phase and water-organic phase transfer hydrogenation, most aryl alkyl ketones can be hydrogenated with the similar results as in homogeneous phase catalytic reaction and with ee about 98%, wherein the expected ω-bromo aryl alkyl alcs. and the epoxy compds. can be obtained from ω-bromo aryl alkyl ketones by the catalytic reaction in aqueous or water-organic two phase medium. The catalysts in the invention can be used to get high conversion rate and unchangeable enantioselectivity even after repeated uses. Surfactants can accelerate this reaction effectively.
IC ICM C07C309-46
ICS C07C303-06; C07C311-18; C07C303-34; C07C029-143; B01J031-12
CC 25-13 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
ST enantioselective prepn benzylic **alc** transfer hydrogenation **chiral** amine
IT Ketones, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(alkyl aromatic; preparation of benzylic **alcs**. and aryl oxiranes via enantioselective transfer hydrogenation of aryl alkyl ketones using water-soluble **chiral** vicinal diamine as ligand)
IT **Alcohols, preparation**
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); **PREP**

(Preparation)
(benzyl; preparation of benzylic **alcs**. and aryl oxiranes via **enantioselective** transfer hydrogenation of aryl alkyl ketones using water-soluble **chiral** vicinal diamine as ligand)

IT Epoxides
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(**chiral**; preparation of benzylic **alcs**. and aryl oxiranes via enantioselective transfer hydrogenation of aryl alkyl ketones using water-soluble **chiral** vicinal diamine as ligand)

IT **Asymmetric synthesis and induction**
Phase transfer catalysts
(preparation of benzylic **alcs**. and aryl oxiranes via enantioselective transfer hydrogenation of aryl alkyl ketones using water-soluble **chiral** vicinal diamine as ligand)

IT Bases, reactions
RL: RGT (Reagent); RACT (Reactant or reagent)
(preparation of benzylic **alcs**. and aryl oxiranes via enantioselective transfer hydrogenation of aryl alkyl ketones using water-soluble **chiral** vicinal diamine as ligand)

IT Hydrogenation
Hydrogenation catalysts
(transfer, stereoselective; preparation of benzylic **alcs**. and aryl oxiranes via enantioselective transfer hydrogenation of aryl alkyl ketones using water-soluble **chiral** vicinal diamine as ligand)

IT 12354-84-6 **37366-09-9** **52462-29-0** **82091-73-4**
RL: **CAT (Catalyst use)**; USES (Uses)
(preparation of benzylic **alcs**. and aryl oxiranes via enantioselective transfer hydrogenation of aryl alkyl ketones using water-soluble **chiral** vicinal diamine as ligand)

IT 76155-80-1P
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of benzylic **alcs**. and aryl oxiranes via enantioselective transfer hydrogenation of aryl alkyl ketones using water-soluble **chiral** vicinal diamine as ligand)

IT 697-64-3P 1517-69-7P 1565-74-8P 20780-54-5P 23357-45-1P 42070-92-8P 52193-85-8P 58287-18-6P 76116-24-0P 86527-10-8P 101219-68-5P 131965-52-1P 162427-79-4P 166239-06-1P
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(preparation of benzylic **alcs**. and aryl oxiranes via enantioselective transfer hydrogenation of aryl alkyl ketones using water-soluble **chiral** vicinal diamine as ligand)

IT 70-11-1 83-33-0 88-15-3 93-08-3 93-55-0 98-59-9, Tosyl chloride 98-86-2, reactions 99-81-0 100-19-6 121-89-1 122-00-9 403-42-9 445-27-2 529-34-0 4254-67-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of benzylic **alcs**. and aryl oxiranes via enantioselective transfer hydrogenation of aryl alkyl ketones using water-soluble **chiral** vicinal diamine as ligand)

L133 ANSWER 23 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:580715 CAPLUS Full-text
DOCUMENT NUMBER: 143:248107
TITLE: Preparation of polymer-supported Ru-TsDPEN catalysts and use for enantioselective synthesis of (S)-fluoxetine
AUTHOR(S): Li, Yangzhou; Li, Zhiming; Li, Feng; Wang, Quanrui; Tao, Fanggang

CORPORATE SOURCE: Department of Chemistry, Fudan University, Shanghai, 200433, Peop. Rep. China
SOURCE: Organic & Biomolecular Chemistry (2005), 3(14), 2513-2518
CODEN: OBCRAK; ISSN: 1477-0520
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 143:248107
ED Entered STN: 06 Jul 2005
AB Polymer-supported chiral ligands were prepared based on Noyori's (1S,2S)- or (1R,2R)-N-(p-tolylsulfonyl)-1,2-diphenylethylenediamine. The combination with [RuCl2(p-cymene)]2 has been shown to exhibit high activities and enantioselectivities for heterogeneous asym. transfer hydrogenation of aromatic ketones with formic acid-triethylamine azeotrope as the hydrogen donor, whereby affording the resp. optically active alcs., the key precursors of chiral fluoxetine. The catalysts can be recovered and reused in three consecutive runs with no significant decline in enantioselectivity. The procedure avoids the plausible contamination of fluoxetine by the toxic transition metal species.
CC 25-7 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
IT **Alcohols, preparation**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of polymer-supported Ru-TsDPEN catalysts for enantioselective synthesis of (**S**)-fluoxetine)
IT **52462-29-0**, p-Cymeneruthenium dichloride dimer 863483-33-4D, polymer-supported
RL: **CAT (Catalyst use)**; USES (Uses)
(preparation of polymer-supported Ru-TsDPEN catalysts for enantioselective synthesis of (S)-fluoxetine)
REFERENCE COUNT: 43 THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L133 ANSWER 24 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:714960 CAPLUS Full-text
DOCUMENT NUMBER: 144:467855
TITLE: Bulky **achiral** triarylphosphines mimic BINAP in Ru(II)-catalyzed asymmetric hydrogenation of ketones
AUTHOR(S): Jing, Qing; Zhang, Xue; Sun, Jie; Ding, Kuiling
CORPORATE SOURCE: State Key Laboratory of Organometallic Chemistry, Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences, Shanghai, 200032, Peop. Rep. China
SOURCE: Advanced Synthesis & Catalysis (2005), 347(9), 1193-1197
CODEN: ASCAF7; ISSN: 1615-4150
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 144:467855
ED Entered STN: 10 Aug 2005
AB Catalysis of the enantioselective hydrogenation of ketones with Ru(II) complexes composed of cheap **achiral** monodentate phosphine ligands in combination with an enantiopure 1,2-diamine, affording a variety of optically active secondary alcs. with high efficiency and enantioselectivity, is reported. The steric impact of **achiral** monophosphine ligands in Ru complexes was found to be a critical factor for the high enantioselectivity of the reaction. This finding throws some light on a long-standing challenge of the

high cost of chiral bisphosphine ligands, associated with an industrial application of the asym. hydrogenation of ketones.

CC 25-7 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 22, 67, 75

ST **chiral** secondary **alc** enantioselective synthesis asym hydrogenation ruthenium catalysis; arom prochiral ketone asym hydrogenation ruthenium catalysis; ruthenium complex **achiral** triarylphosphine **chiral** diamine crystal mol structure; mol mechanics ruthenium complex steric hindrance **achiral** triarylphosphine ligand

IT Steric hindrance
(effect of steric hindrance of **achiral** triarylphosphine ligands on the enantioselectivity of asym. hydrogenation of ketones catalyzed by Ru(II) complexes)

IT Molecular mechanics
(mol. structure of a Ru(II) complex with an **achiral** triarylphosphine ligand and a chiral diamine calculated by mol. mechanics)

IT Molecular structure
(of Ru(II) complexes with **achiral** triarylphosphine ligands and a chiral diamine)

IT Transition metal complexes
RL: CAT (Catalyst use); PRP (Properties); USES (Uses)
(phosphine; preparation of **chiral** secondary **alcs**. via asym. hydrogenation of ketones catalyzed by Ru(II) complexes with bulky **achiral** triarylphosphine ligands and a **chiral** diamine)

IT **Asymmetric synthesis and induction**
(preparation of **chiral** secondary **alcs**. via asym. hydrogenation of ketones catalyzed by Ru(II) complexes with bulky **achiral** triarylphosphine ligands and a **chiral** diamine)

IT Ketones, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(prochiral, aromatic prochiral ketones; preparation of **chiral** secondary **alcs**. via asym. hydrogenation of ketones catalyzed by Ru(II) complexes with bulky **achiral** triarylphosphine ligands and a **chiral** diamine)

IT **Alcohols, preparation**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(secondary, **chiral**; preparation of **chiral** secondary **alcs**. via asym. hydrogenation of ketones catalyzed by Ru(II) complexes with bulky **achiral** triarylphosphine ligands and a **chiral** diamine)

IT Hydrogenation
Hydrogenation catalysts
(stereoselective; preparation of **chiral** secondary **alcs**. via asym. hydrogenation of ketones catalyzed by Ru(II) complexes with bulky **achiral** triarylphosphine ligands and a **chiral** diamine)

IT Phosphines
RL: CAT (Catalyst use); PRP (Properties); USES (Uses)
(transition metal complexes; preparation of **chiral** secondary **alcs**. via asym. hydrogenation of ketones catalyzed by Ru(II) complexes with bulky **achiral** triarylphosphine ligands and a **chiral** diamine)

IT **886446-25-9 886446-34-0**
RL: **CAT (Catalyst use)**; PRP (Properties); USES (Uses)
(crystal structure; preparation of **chiral** secondary **alcs** . via asym. hydrogenation of ketones catalyzed by Ru(II) complexes with bulky **achiral** triarylphosphine ligands and a **chiral**

diamine)

IT **886446-37-3**
RL: **CAT (Catalyst use)**; PRP (Properties); USES (Uses)
(mol. structure calculated by mol. mechanics; preparation of **chiral** secondary **alcs**. via asym. hydrogenation of ketones catalyzed by Ru(II) complexes with bulky **achiral** triarylphosphine ligands and a **chiral** diamine)

IT **886446-26-0 886446-36-2**
RL: **CAT (Catalyst use)**; USES (Uses)
(preparation of **chiral** secondary **alcs**. via asym. hydrogenation of ketones catalyzed by Ru(II) complexes with bulky **achiral** triarylphosphine ligands and a **chiral** diamine)

IT 88-15-3, 2-Thienyl methyl ketone 93-08-3 93-55-0, Ethyl phenyl ketone 98-80-6, Phenylboric acid 98-86-2, Methyl phenyl ketone, reactions 99-02-5 100-06-1, Methyl 4-methoxyphenyl ketone 122-00-9, Methyl 4-methylphenyl ketone 403-42-9 445-27-2 577-16-2, Methyl 2-methylphenyl ketone 579-74-8, Methyl 2-methoxyphenyl ketone 626-39-1, 1,3,5-Tribromobenzene 941-98-0, 1-Naphthyl methyl ketone 1192-62-7, 2-Furyl methyl ketone 1271-55-2, Ferrocenyl methyl ketone 2142-63-4 2142-68-9 2142-69-0 3506-36-3 17408-14-9 30071-93-3 172975-69-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of **chiral** secondary **alcs**. via asym. hydrogenation of ketones catalyzed by Ru(II) complexes with bulky **achiral** triarylphosphine ligands and a **chiral** diamine)

IT 103068-20-8P 278600-38-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of **chiral** secondary **alcs**. via asym. hydrogenation of ketones catalyzed by Ru(II) complexes with bulky **achiral** triarylphosphine ligands and a **chiral** diamine)

IT 7719-12-2, Phosphorus trichloride
RL: RGT (Reagent); RACT (Reactant or reagent)
(preparation of **chiral** secondary **alcs**. via asym. hydrogenation of ketones catalyzed by Ru(II) complexes with bulky **achiral** triarylphosphine ligands and a **chiral** diamine)

IT 613-87-6P, (S)-1-Phenyl propanol 1445-91-6P, (S)-1-Phenyl ethanol 1572-97-0P, (S)-1-(4-MethoxyPhenyl) ethanol 15914-84-8P, (S)-1-(1-Naphthyl) ethanol 27544-18-9P, (S)-1-(2-Naphthyl) ethanol 27948-39-6P, (S)-1-(2-Thienyl) ethanol 33136-66-2P 36296-97-6P 51100-05-1P, (S)-1-(2-MethylPhenyl) ethanol 51154-54-2P, (S)-1-(4-MethylPhenyl) ethanol 101219-73-2P, (S)-1-(4-FluoroPhenyl) ethanol 108100-06-7P, (S)-1-(2-MethoxyPhenyl) ethanol 112653-32-4P, (S)-1-(2-Furyl) ethanol 114446-55-8P, (S)-1-(2-BromoPhenyl) ethanol 127852-27-1P, (S)-1-(2-TrifluoromethylPhenyl) ethanol 131864-71-6P, (S)-1-(2-ChloroPhenyl) ethanol 134615-22-8P, (S)-1-(3-BromoPhenyl) ethanol 135145-34-5P, (S)-1-(3-ChloroPhenyl) ethanol 171032-87-4P, (S)-1-(2-FluoroPhenyl) ethanol 225920-05-8P, (S)-1-[3,5-Bis(Trifluoromethyl)Phenyl] ethanol 561068-06-2P 886232-53-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of **chiral** secondary **alcs**. via asym. hydrogenation of ketones catalyzed by Ru(II) complexes with bulky **achiral** triarylphosphine ligands and a **chiral** diamine)

IT 67-63-0, Iso-propanol, uses
RL: NUU (Other use, unclassified); USES (Uses)

(solvent; preparation of **chiral** secondary **alcs.** via asym. hydrogenation of ketones catalyzed by Ru(II) complexes with bulky **achiral** triarylphosphine ligands and a **chiral** diamine)

REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

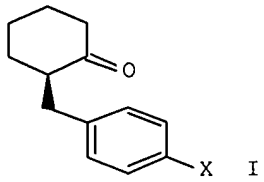
L133 ANSWER 25 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:6908 CAPLUS Full-text
DOCUMENT NUMBER: 145:418744
TITLE: The synthesis of ortho-keto-substituted N,N-dimethyl-(S)-1-phenethylamines
AUTHOR(S): Shishkina, I. N.; Kuznetsova, A. A.; Demyanovich, V. M.; Potekhin, K. A.
CORPORATE SOURCE: Kafedra Org. Khim., Mosk. Gos. Univ., Moscow, Russia
SOURCE: Vestnik Moskovskogo Universiteta, Seriya 2: Khimiya (2005), 46(5), 345-348
CODEN: VMUKA5; ISSN: 0579-9384
PUBLISHER: Izdatel'stvo Moskovskogo Universiteta
DOCUMENT TYPE: Journal
LANGUAGE: Russian
OTHER SOURCE(S): CASREACT 145:418744
ED Entered STN: 05 Jan 2006

AB A series of (S)-o-acyl-α,N,N-trimethylbenzylamines (acyl = benzoyl, pivaloyl, p-toluoyl, etc.) were synthesized by condensation of ortho-lithiated (S)-α,N,N-trimethylbenzylamine with the corresponding acyl chlorides. Three methods for the reduction of the resulting amino ketones, i.e. with LiAlH4, with LiAlH(OBu-t)3 or with D-tartaric acid-modified NaBH4, were investigated; the latter method is shown to be superior for the diastereomeric purity of the products. The amino alcs. prepared were used as chiral catalysts in enantioselective addition of Et2Zn to benzaldehyde providing (R)-1-phenylethanol in 35-79% ee's.

CC 25-16 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
ST ketone amino prepn redn; amino **alc** prepn **chiral** catalyst asym addn diethylzinc benzaldehyde; phenylethylamine ortho lithiation acylation acyl chloride
IT **Ketones, preparation**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(amino; preparation of non-**racemic** ortho-acyl-α,N,N-trimethylbenzylamines by ortho-lithiation of α,N,N-trimethylbenzylamine followed by trapping with acyl chlorides)
IT **Alcohols, preparation**
RL: CAT (Catalyst use); SPN (Synthetic preparation); **PREP (Preparation)**; USES (Uses)
(amino; preparation of ortho-(hydroxyalkyl)-α,N,N-trimethylbenzylamines by reduction of non-racemic o-acyl-α,N,N-trimethylbenzylamines and their use as catalysts for asym. addition of diethylzinc to benzaldehyde)
IT **Asymmetric synthesis and induction**
(preparation of ortho-(hydroxyalkyl)-α,N,N-trimethylbenzylamines by reduction of non-racemic o-acyl-α,N,N-trimethylbenzylamines and their use as catalysts for asym. addition of diethylzinc to benzaldehyde)

L133 ANSWER 26 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:127619 CAPLUS Full-text
DOCUMENT NUMBER: 142:373286
TITLE: A Chiral Cyclohexanone Linked to Polystyrene for Solid-Phase Synthesis of Chiral α-Carbonyls

AUTHOR(S): Spino, Claude; Gund, Vitthal Genbhau; Nadeau, Christian
CORPORATE SOURCE: Departement of Chimie, Universite of Sherbrooke, Sherbrooke, QC, J1K 2R1, Can.
SOURCE: Journal of Combinatorial Chemistry (2005), 7(2), 345-352
CODEN: JCCHFF; ISSN: 1520-4766
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 142:373286
ED Entered STN: 15 Feb 2005
GI



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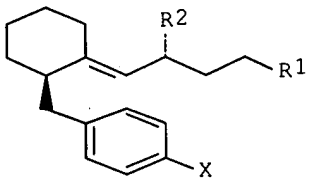


II

AB Two chiral cyclohexanones were linked to polystyrene resin. The polymer-bound auxiliaries were subjected to a sequence of four reactions, the last of which cleaves the desired α-chiral carbonyl compound off the resin, concurrently regenerating the resin-bound auxiliary in its original form. Thus, addition of vinyllithiums, derived from alkenyl iodides R1CH2CH2CH:CHI (R1 = n-Pr, Ph, Me3CSiMe2O), to the resin-bound cyclohexanone I (X = resin) followed by chloroformylation / cuprate addition gave the resin-bound alkylidenecyclohexanes II (R2 = Me, Me3C, Ph, 1-naphthyl, etc.), which were cleaved by ozonation to give, after reduction of oxidation if required, a set of non-racemic alcs., aldehydes and carboxylic acids ZCHR2CH2CH2R1 (Z = HOCH2, CHO, HO2C). The resin can then be reused.
CC 21-2 (General Organic Chemistry)
ST cyclohexanone polystyrene linked **chiral** auxiliary carbonyl compd asym synthesis; aldehyde branched solid phase asym synthesis; **alc** branched solid phase asym synthesis; carboxylic acid branched solid phase asym synthesis
IT Carboxylic acids, preparation
RL: SPN (Synthetic preparation); PREP (Preparation)
(aliphatic; asym. solution and solid-phase synthesis of branched **alcs**., aldehydes and carboxylic acids using non-racemic cyclohexanones as **chiral** auxiliaries)
IT **Asymmetric synthesis and induction**
Chiral auxiliary
Solid phase synthesis
(asym. solution and solid-phase synthesis of branched **alcs**., aldehydes and carboxylic acids using non-racemic cyclohexanones as **chiral** auxiliaries)
IT Aldehydes, preparation
RL: SPN (Synthetic preparation); PREP (Preparation)
(asym. solution and solid-phase synthesis of branched **alcs**., aldehydes and carboxylic acids using non-racemic cyclohexanones as **chiral** auxiliaries)
IT **Alcohols, preparation**
RL: SPN (Synthetic preparation); **PREP (Preparation)**

(**chiral**; asym. solution and solid-phase synthesis of branched **alcs.**, aldehydes and carboxylic acids using non-racemic cyclohexanones as **chiral** auxiliaries)

IT **Ketones, preparation**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(cycloalkanones; asym. solution and solid-phase synthesis of branched **alcs.**, aldehydes and carboxylic acids using non-**racemic** cyclohexanones as **chiral** auxiliaries)

IT Alkylation
(stereoselective; asym. solution and solid-phase synthesis of branched **alcs.**, aldehydes and carboxylic acids using non-racemic cyclohexanones as **chiral** auxiliaries)

IT 1119-51-3, 5-Bromo-1-pentene 2398-37-0, 3-Methoxyphenyl bromide
RL: RCT (Reactant); RACT (Reactant or reagent)
(Grignard preparation; asym. solution and solid-phase synthesis of branched **alcs.**, aldehydes and carboxylic acids using non-racemic cyclohexanones as **chiral** auxiliaries)

IT 98-80-6, Phenylboronic acid 108-86-1, Bromobenzene, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(Suzuki coupling; asym. solution and solid-phase synthesis of branched **alcs.**, aldehydes and carboxylic acids using non-racemic cyclohexanones as **chiral** auxiliaries)

IT 77857-39-7P
RL: BYP (Byproduct); PREP (Preparation)
(asym. solution and solid-phase synthesis of branched **alcs.**, aldehydes and carboxylic acids using non-racemic cyclohexanones as **chiral** auxiliaries)

IT 89-82-7, (+)-Pulegone 94-66-6, 2-Allylcyclohexanone 589-15-1, 4-Bromobenzyl bromide 24347-58-8 25015-63-8, Pinacolborane 77857-35-3 106380-46-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(asym. solution and solid-phase synthesis of branched **alcs.**, aldehydes and carboxylic acids using non-racemic cyclohexanones as **chiral** auxiliaries)

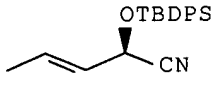
IT 53045-12-8P 60595-37-1P, (E)-1-Iodo-1-heptene 67074-37-7P 77857-39-7DP, polystyrene-supported 108330-00-3P 184370-59-0P 322640-09-5P 849435-82-1P 849435-83-2P 849435-84-3P 849435-85-4P 849435-88-7P 849435-89-8P 849435-90-1P 849435-91-2P 849435-93-4P 849435-94-5P 849435-95-6P 849435-96-7P 849435-97-8P 849435-98-9P 849435-99-0P 849436-01-7P 849436-03-9P 849436-04-0P 849436-10-8P 849436-21-1P 849436-25-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(asym. solution and solid-phase synthesis of branched **alcs.**, aldehydes and carboxylic acids using non-racemic cyclohexanones as **chiral** auxiliaries)

IT 122-97-4P, 3-Phenyl-1-propanol 1949-41-3P 3023-61-8P 17296-92-3P 17297-03-9P 21490-50-6P 40654-82-8P 80651-37-2P 101711-91-5P 128441-03-2P 194922-80-0P 356784-34-4P 494844-20-1P 849435-86-5P 849435-87-6P 849435-92-3P 849436-00-6P 849436-02-8P 849436-05-1P 849436-06-2P 849436-07-3P 849436-08-4P 849436-09-5P 849436-11-9P 849436-12-0P 849436-13-1P 849436-14-2P 849436-15-3P 849436-16-4P 849436-17-5P 849436-18-6P 849436-19-7P 849436-20-0P 849436-22-2P 849436-23-3P 849436-24-4P 849487-55-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(asym. solution and solid-phase synthesis of branched **alcs.**, aldehydes and carboxylic acids using non-racemic cyclohexanones as **chiral** auxiliaries)

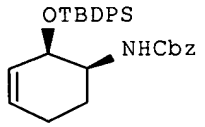
IT 628-71-7, 1-Heptyne 1823-14-9, 5-Phenyl-1-pentyne 78592-82-2

218434-90-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(hydroiodination; asym. solution and solid-phase synthesis of branched **alcs.**, aldehydes and carboxylic acids using non-racemic cyclohexanones as **chiral** auxiliaries)
REFERENCE COUNT: 54 THERE ARE 54 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

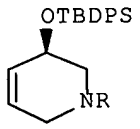
L133 ANSWER 27 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:831386 CAPLUS Full-text
DOCUMENT NUMBER: 142:38128
TITLE: Conversion of chiral unsaturated cyanohydrins into chiral carba- and heterocycles via ring-closing metathesis
AUTHOR(S): van den Nieuwendijk, Adrianus M. C. H.; Ghisaidoobe, Amar B. T.; Overkleeft, Herman S.; Brussee, Johannes; van der Gen, Arne
CORPORATE SOURCE: Leiden Institute of Chemistry, Gorlaeus Laboratories, Leiden University, Leiden, 2300 RA, Neth.
SOURCE: Tetrahedron (2004), 60(46), 10385-10396
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 142:38128
ED Entered STN: 12 Oct 2004
GI



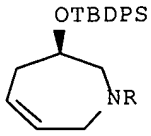
I



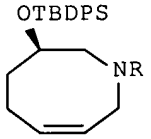
II



III



IV



V

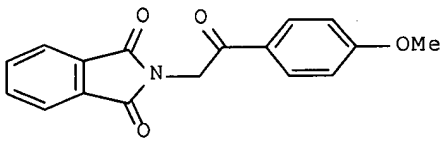
AB Aliphatic unsatd. cyanohydrins, e.g., I, served as starting materials in the synthesis of a set of new chiral unsatd. cyclic 1,2-ethanolamines. Combining a Grignard addition-NaBH4 reduction sequence with a ring-closing metathesis afforded unsatd. cyclic 1,2-ethanolamines, e.g., II, in good yields and high ee (96-99%). The conversion of cyanohydrins via a DIBAL reduction-transimination-NaBH4 reduction sequence, using allylamine, followed by ring-closing metathesis yielded tetrahydropyridines III (R = Cbz, Boc, Bn), tetrahydroazepinols IV and tetrahydroazocinols V (R = Cbz, Boc) in high yields and excellent ee (97-99%).
CC 27-21 (Heterocyclic Compounds (One Hetero Atom))
IT **Alcohols, preparation**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(amino, cyclic chiral; stereoselective preparation of chiral unsatd. cyclic ethanolamines via Grignard addition to chiral silylcyanohydrins followed by in situ reduction and N-protection with subsequent ring-closing

metathesis catalyzed by Grubb's catalyst)

IT 172222-30-9
RL: **CAT (Catalyst use)**; USES (Uses)
(stereoselective preparation of chiral unsatd. cyclic ethanolamines via Grignard addition to chiral silylcyanohydrins followed by in situ reduction and N-protection with subsequent ring-closing metathesis catalyzed by Grubb's catalyst)

REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L133 ANSWER 28 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:61086 CAPLUS Full-text
DOCUMENT NUMBER: 140:235450
TITLE: Highly Enantioselective Asymmetric Hydrogenation of α-Phthalimide Ketone: An Efficient Entry to Enantiomerically Pure Amino Alcohols
AUTHOR(S): Lei, Aiwen; Wu, Shulin; He, Minsheng; Zhang, Xumu
CORPORATE SOURCE: Department of Chemistry, Pennsylvania State University, University Park, PA, 16802, USA
SOURCE: Journal of the American Chemical Society (2004), 126(6), 1626-1627
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 140:235450
ED Entered STN: 26 Jan 2004
GI



I

AB A new type of α-phthalimide ketones, e.g. I, was hydrogenated in excellent enantioselectivity by using a Ru-(C3-TunePhos) complex as the catalyst. Up to 10 000 turnovers have been achieved in more than 99% ee in the hydrogenation reaction. A dynamic kinetic resolution study for the synthesis of threonine was performed, and high anti selectivity (>97:3) was observed for the first time. An efficient method to synthesize enantiomerically pure amino alcs. has been developed.

CC 25-8 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)

IT **Alcohols, preparation**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(amino; preparation of amino alcs. via Ru-catalyzed enantioselective asym. hydrogenation of α-phthalimide ketone)

IT **Resolution (separation)**
(**kinetic, dynamic**; formation of optically pure allo-threonine derivs. via Ru-catalyzed enantioselective asym. hydrogenation of α-phthalimide ketone)

IT 503114-19-0 668422-82-0
RL: **CAT (Catalyst use)**; USES (Uses)
(preparation of amino alcs. via Ru-catalyzed enantioselective asym. hydrogenation of α-phthalimide ketone)

REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L133 ANSWER 29 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:846735 CAPLUS Full-text
DOCUMENT NUMBER: 142:354931
TITLE: A convenient synthesis of optically active unhindered aliphatic alcohols with high optical purity from non-racemic β-hydroxy sulfides
AUTHOR(S): Cho, Byung Tae; Kim, Dong Jun
CORPORATE SOURCE: Department of Chemistry, Hallym University, Chunchon, 200-702, S. Korea
SOURCE: Bulletin of the Korean Chemical Society (2004), 25(9), 1385-1391
CODEN: BKCSDE; ISSN: 0253-2964
PUBLISHER: Korean Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 142:354931
ED Entered STN: 15 Oct 2004
AB A general route for the synthesis of optically active unhindered aliphatic alcs., where the steric demands between two alkyl groups adjacent to the carbinol are similar, with high enantiomeric purity has been developed by sulfoxidn. of chiral β-hydroxy sulfides, followed by alkylation and desulfurization.
CC 23-7 (Aliphatic Compounds)
IT **Alcohols, preparation**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(aliphatic; synthesis of optically active unhindered aliphatic alcs. with high optical purity from non-racemic β-hydroxy sulfides)
IT **Asymmetric synthesis and induction**
Reduction
(synthesis of optically active unhindered aliphatic alcs. with high optical purity from non-racemic β-hydroxy sulfides)
IT **Ketones, reactions**
RL: RCT (Reactant); RACT (Reactant or reagent)
(synthesis of optically active unhindered aliphatic alcs. with high optical purity from non-**racemic** β-hydroxy sulfides)
REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L133 ANSWER 30 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:70318 CAPLUS Full-text
DOCUMENT NUMBER: 140:253304
TITLE: Palladium-catalyzed oxidative kinetic resolution with ambient air as the stoichiometric oxidation gas
AUTHOR(S): Bagdanoff, Jeffrey T.; Stoltz, Brian M.
CORPORATE SOURCE: The Arnold and Mabel Beckman Laboratories of Chemical Synthesis, Division of Chemistry and Chemical Engineering, California Institute of Technology, Pasadena, CA, 91125, USA
SOURCE: Angewandte Chemie, International Edition (2004), 43(3), 353-357
CODEN: ACIEF5; ISSN: 1433-7851
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 140:253304
ED Entered STN: 29 Jan 2004

AB Air was enough to mediate the enantioselective oxidation of secondary alcs. at room temperature with palladium(II) and sparteine in nonflammable solvents. Examination of the role of solvents capable of hydrogen bonding and their ability to solvate halide anions, led to a set of conditions for the enantioselective oxidative kinetic resolution of secondary alcs.

CC 25-16 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 75, 78

ST **alc** oxidative kinetic resoln; ketone prepn; **chiral** **alc** prepn; palladium oxidative kinetic resoln catalyst

IT **Ketones, preparation**
RL: SPN (Synthetic preparation); PREP (Preparation)
(aromatic; preparation of ketones via palladium-catalyzed oxidative kinetic resolution of **racemic** alcs.)

IT **Resolution (separation)**
(kinetic, oxidative; stereoselective preparation of alcs. via palladium-catalyzed oxidative kinetic resolution of racemic alcs.)

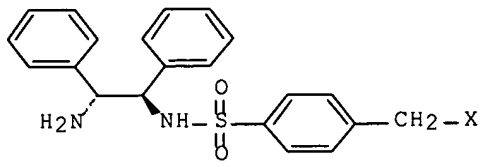
IT **Alcohols, preparation**
RL: PUR (Purification or recovery); SPN (Synthetic preparation); **PREP (Preparation)**
(secondary, **chiral**; stereoselective preparation of **alcs.** via palladium-catalyzed oxidative kinetic resolution of racemic **alcs.**)

IT **Asymmetric synthesis and induction**
(stereoselective preparation of alcs. via palladium-catalyzed oxidative kinetic resolution of racemic alcs.)

IT 1517-69-7, (+)-1-Phenylethanol
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of acetophenone via palladium-catalyzed oxidation of **chiral** phenylethanol in the evaluation of solvents for the oxidative kinetic resolution of racemic **alcs.**)

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L133 ANSWER 31 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:995754 CAPLUS Full-text
DOCUMENT NUMBER: 140:163517
TITLE: Efficient Heterogeneous Asymmetric Transfer Hydrogenation of Ketones Using Highly Recyclable and Accessible Silica-Immobilized Ru-TsDPEN Catalysts
AUTHOR(S): Liu, Pei Nian; Gu, Pei Ming; Wang, Fei; Tu, Yong Qiang
CORPORATE SOURCE: Department of Chemistry and State Key Laboratory of Applied Organic Chemistry, Lanzhou University, Lanzhou, 730000, Peop. Rep. China
SOURCE: Organic Letters (2004), 6(2), 169-172
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 140:163517
ED Entered STN: 23 Dec 2003
GI



I

AB Chiral Ru-TsDPEN [N-(p-toluenesulfonyl)-1,2-diphenylethylenediamine] (I, X = H)-derived catalysts were first successfully immobilized onto amorphous silica gel and mesoporous silicas of MCM-41 and SBA-15 by an easily accessible approach. The silica-immobilized catalyst (I; X = CH2-Silica) demonstrated remarkably high catalytic activities and excellent enantioselectivities (up to >99% ee) for the heterogeneous asym. transfer hydrogenation of various ketones. Particularly, the catalyst could be readily recovered and reused in multiple consecutive catalytic runs (up to 10 uses) with the completely maintained enantioselectivity.

CC 25-7 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)

ST arom ketone asym transfer hydrogenation **chiral** ruthenium; **alc** secondary arom enantioselective prepn; asym transfer hydrogenation catalyst ruthenium **chiral** toluenesulfonyldiphenylethylenediamine silica immobilization

IT Ketones, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(aromatic; enantioselective preparation of aromatic **alcs**. via asym. transfer hydrogenation of aromatic ketones catalyzed by silica-immobilized **chiral** Ru-TsDPEN complexes)

IT **Asymmetric synthesis and induction**
(enantioselective preparation of aromatic **alcs**. via asym. transfer hydrogenation of aromatic ketones catalyzed by silica-immobilized **chiral** Ru-TsDPEN complexes)

IT **Alcohols, preparation**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(secondary, **chiral**, aromatic; **enantioselective** preparation of aromatic **alcs**. via asym. transfer hydrogenation of aromatic ketones catalyzed by silica-immobilized **chiral** Ru-TsDPEN complexes)

IT Hydrogenation
Hydrogenation catalysts
(transfer, stereoselective; enantioselective preparation of aromatic **alcs**. via asym. transfer hydrogenation of aromatic ketones catalyzed by silica-immobilized **chiral** Ru-TsDPEN complexes)

IT **52462-29-0**
RL: **CAT (Catalyst use)**; USES (Uses)
(enantioselective preparation of aromatic **alcs**. via asym. transfer hydrogenation of aromatic ketones catalyzed by silica-immobilized **chiral** Ru-TsDPEN complexes)

IT 144222-34-4DP, silica-bound
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(enantioselective preparation of aromatic **alcs**. via asym. transfer hydrogenation of aromatic ketones catalyzed by silica-immobilized **chiral** Ru-TsDPEN complexes)

IT 83-33-0, 1-Indanone 93-08-3 98-86-2, Acetophenone, reactions 445-27-2, 2'-Fluoroacetophenone 455-36-7 529-34-0, 1-Tetralone 586-37-8 614-16-4, α-Cyanoacetophenone 1192-62-7, 2-Furylmethylketone 2142-68-9, 2'-Chloroacetophenone 2142-69-0,

2'-Bromoacetophenone
RL: RCT (Reactant); RACT (Reactant or reagent)
(enantioselective preparation of aromatic **alcs.** via asym. transfer hydrogenation of aromatic ketones catalyzed by silica-immobilized **chiral** Ru-TsDPEN complexes)

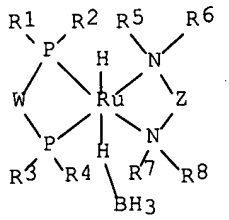
IT 697-64-3P 1517-69-7P 23357-45-1P 27948-61-4P 52193-85-8P 73627-97-1P 76116-20-6P 120466-66-2P 120523-12-8P 126534-33-6P 162427-79-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(enantioselective preparation of aromatic **alcs.** via asym. transfer hydrogenation of aromatic ketones catalyzed by silica-immobilized **chiral** Ru-TsDPEN complexes)

REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L133 ANSWER 32 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:277075 CAPLUS Full-text
DOCUMENT NUMBER: 138:304045
TITLE: Preparation of ruthenium diphosphine diamine hydride complexes and preparation of alcohols under base-free conditions and optical resolution of racemic carbonyl compounds using the prepared ruthenium hydride complexes
INVENTOR(S): Okuma, Takeshi; Koizumi, Masatoshi; Muniz, Kilian; Noyori, Ryoji
PATENT ASSIGNEE(S): Nagoya Sangyo Kagaku Kenkyusho, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 14 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2003104993	A	20030409	JP 2001-301852	20010928
US 6720439	B1	20040413	US 2002-291611	20021112
PRIORITY APPLN. INFO.:			JP 2001-301852 A	20010928

OTHER SOURCE(S): MARPAT 138:304045
ED Entered STN: 10 Apr 2003
GI



I

AB The title complexes I [W = (un)substituted binaphthyl connected to P at 2- or 2'-position; R1-R4 = (un)substituted hydrocarbyl; R1R2 and/or R3R4 may form ring; R5-R8 = H, (un)substituted hydrocarbyl; Z = (un)substituted hydrocarbyl] are prepared Alcs. are prepared by reduction of carbonyl compds. with H or with H donors in the presence of Ru hydride complexes in the absence of strong

bases. Racemic carbonyl compds. are optically resolved by selective reduction of one enantiomer in the presence of Ru hydride complexes. Thus, acetophenone was hydrogenated with H in the presence of {trans-RuH(η1-BH4)[(S)-xylbinap][(S,S)-dpen]} [(S)-xylbinap = (S)-2,2'-bis(di-3,5-xylylphosphino)-1,1'-binaphthyl, (S,S)-dpen = (S,S)-1,2-diphenylethylenediamine] in i-PrOH at 25° for 12 h to give 95% (R)-1-phenylethanol with 99% e.e.

IC ICM C07F009-50
ICS B01J031-24; C07B041-02; C07C029-145; C07C033-03; C07C033-22; C07C035-08; C07C041-26; C07C041-44; C07C043-196; C07C045-85; C07C049-403; C07C067-31; C07C069-732; C07C069-84; C07C211-27; C07C213-00; C07C215-30; C07D301-00; C07D301-32

CC 25-7 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 29, 67

IT **Ketones, reactions**
RL: RCT (Reactant); RACT (Reactant or reagent)
(amino; optical resolution of **racemic** carbonyl compds. by reduction using Ru diphosphine diamine hydride complexes)

IT **Alcohols, preparation**
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); **PREP (Preparation)**
(**chiral**; preparation of **alcs**. by hydrogenation of carbonyl compds. using Ru diphosphine diamine hydride complex catalysts)

IT **Ketones, preparation**
RL: PUR (Purification or recovery); PREP (Preparation)
(optical resolution of **racemic** carbonyl compds. by reduction using Ru diphosphine diamine hydride complexes)

L133 ANSWER 33 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:509919 CAPLUS Full-text
DOCUMENT NUMBER: 139:77882
TITLE: Novel ruthenium complexes and process for preparing alcoholic compounds using these
INVENTOR(S): Kunihiko, Tsutsumi; Kunihiko, Murata; Takeshi, Ota; Takao, Ikariya
PATENT ASSIGNEE(S): Kanto Kagaku Kabushiki Kaisha, Japan
SOURCE: Eur. Pat. Appl., 28 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1323724	A2	20030702	EP 2002-28791	20021223
EP 1323724	A3	20030924		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
JP 2003252884	A	20030910	JP 2002-248058	20020828
JP 3566955	B2	20040915		
CA 2414265	A1	20030628	CA 2002-2414265	20021216
US 2003166978	A1	20030904	US 2002-330501	20021227
US 6790973	B2	20040914		

PRIORITY APPLN. INFO.: JP 2001-401170 A 20011228
JP 2002-248058 A 20020828

OTHER SOURCE(S): MARPAT 139:77882
ED Entered STN: 04 Jul 2003
AB Claimed are optically active Ru diphosphine complexes which have asymmetry on carbon, Ru(X)(Y)(R5R6PCHR1CR3R4CHR2PR7R8) (1, wherein X and Y represent a H

atom or an anion group, R1 and R2 represent a chain or cyclic hydrocarbon C1-20 group which can be substituted, R3 and R4 represent a H atom or a hydrocarbon C1-3 group, and R5, R6, R7 and R8 represent a hydrocarbon C1-30 group which can be substituted, with the proviso that when X and Y are Br, R1 and R2 are a Me group, and when R3 and R4 are a H atom, at least one of R5, R6, R7 and R8 is not a Ph group.), and optically active Ru diphosphine diamine complexes Ru(X)(Y)(R5R6PCHR1CR3R4CHR2PR7R8)(R9R10NCR13R14-Z-CR15R16NR11R12) where X, Y and diphosphine are as above and chiral diamine is, e.g., daipen (1-isopropyl-2,2-bis(p-methoxyphenyl)ethylenediamine). A process for enantioselectively preparing an alc. is provided whereby a carbonyl compound is reduced with H2 in the presence of 1 as catalyst. This asym. hydrogenation process has excellent results in terms of reactivity and enantioselectivity when compared with conventional Ru catalysts having an optically active diphosphine compound having the axial chirality or the asymmetry on C as the ligand. Thus, [RuBr2{(S,S)-Tolskewphos}{(R)-daipen}] [2, Tolskewphos = 2,4-bis(di-4-tolylphosphino)pentane] was prepared via [Ru{(S,S)-Tolskewphos}{methylallyl}] and [RuBr2{(S,S)-Tolskewphos}] intermediates. Asym. hydrogenation of acetophenone catalyzed by 2 in 2-propanol with added KOCMe3 as base afforded (R)-phenethyl alc. in ≥99% yield and 93.8% e.e.

IC ICM C07F015-00
ICS C07C029-145; C07C029-14

CC 78-7 (Inorganic Chemicals and Reactions)
Section cross-reference(s): 21

IT **Asymmetric synthesis and induction**
(enantioselective hydrogenation of carbonyl compds. to alcs. catalyzed by optically active ruthenium diphosphine complexes)

IT **Alcohols, preparation**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(**enantioselective** hydrogenation of carbonyl compds. to alcs. catalyzed by optically active ruthenium diphosphine complexes)

IT **551950-95-9 551950-96-0**
RL: **CAT (Catalyst use)**; USES (Uses)
(asym. hydrogenation of carbonyl compds. to alcs. catalyzed by optically active ruthenium diphosphine complexes)

IT **329735-86-6 329736-05-2 551950-89-1**
552289-74-4
RL: **CAT (Catalyst use)**; USES (Uses)
(optically active catalyst for asym. hydrogenation of carbonyl compds. to alcs.)

IT **551950-86-8P 551950-90-4P 551950-94-8P**
552289-81-3P
RL: **CAT (Catalyst use)**; SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(preparation as optically active catalyst for asym. hydrogenation of carbonyl compds. to alcs.)

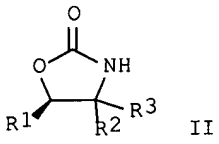
IT **551950-88-0P 551950-93-7P**
RL: **CAT (Catalyst use)**; RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation, coordinative addition of **chiral** diamine, and optically active catalyst for asym. hydrogenation of carbonyl compds. to **alcs.**)

L133 ANSWER 34 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:707996 CAPLUS Full-text
DOCUMENT NUMBER: 139:307568
TITLE: Rapid racemization of chiral non-racemic sec-alcohols catalyzed by (η5-C5(CH3)5)Ru complexes bearing tertiary phosphine-primary amine chelate ligands
AUTHOR(S): Ito, Masato; Osaku, Akihide; Kitahara, Sachiko; Hirakawa, Makoto; Ikariya, Takao

CORPORATE SOURCE: Tokyo Institute of Technology, Frontier Collaborative Research Center, Department of Applied Chemistry, Graduate School of Science and Engineering, Meguro-ku, Tokyo, 152-8552, Japan
SOURCE: Tetrahedron Letters (2003), 44(40), 7521-7523
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 139:307568
ED Entered STN: 10 Sep 2003
AB A ternary catalyst system of chloro[(1,2,5,6-η)-1,5-cyclooctadiene][(1,2,3,4,5-η)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien- 1-yl]ruthenium, 2-(diphenylphosphino)ethanamine and potassium tert-butoxide causes rapid racemization of chiral non-racemic sec-alcs., which results from the reversible hydrogen transfer between sec-alcs. and ketones. Other ligands thus screened included N,N-dimethyl-1,2- ethanediamine, 2-(diphenylphosphino)-N-methylethanamine, 2-(diphenylphosphino)-N,N-dimethylethanamine, 2-(phenylthio)ethanamine, 3-(diphenylphosphino)-1-propanamine, 2-(diphenylphosphino)benzenemethanami ne. Both tertiary phosphine and primary amine functionalities in the ligand are responsible for the high rate. The role of solvents in this reaction was examined; the reaction of (αR)-α-methylbenzenemethanol in acetone as solvent yielded acetophenone, instead of (±)-α-methylbenzenemethanol, suggesting the intermediate formation of ketones. Isotope labeling expts. were also reported. In view of recent advances in dynamic kinetic resolution of racemic secondary alcs. in which the transition metal-catalyzed racemization is coupled with an enzymic transformation of alcs., the above catalyst system may also contribute to the dynamic kinetic resolution, since it exhibits a high catalyst performance under conditions favorable for enzymic reactions.
CC 25-7 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
IT **Resolution (separation)**
(**kinetic, dynamic kinetic** resolution;
racemization of chiral sec-alcs. catalyzed by chloro[cyclooctadiene][pentamethylcyclopentadienyl]ruthenium/(diphenylphosphino)ethanamine in presence of potassium tert-butoxide)
IT **Alcohols, preparation**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(secondary, racemic secondary alcs.; racemization of chiral sec-alcs. catalyzed by chloro[cyclooctadiene][pentamethylcyclopentadienyl]ruthenium/(diphenylphosphino)ethanamine in presence of potassium tert-butoxide)
IT 108-00-9, N,N-Dimethyl-1,2-ethanediamine 865-47-4 2014-75-7, 2-(Phenylthio)ethanamine 4848-43-5, 2-(Diphenylphosphino)ethanamine 16605-03-1, 3-(Diphenylphosphino)-1-propanamine 29679-67-2, 2-(Diphenylphosphino)-N,N-dimethylethanamine **92390-26-6**, Chloro[(1,2,5,6-η)-1,5-cyclooctadiene][(1,2,3,4,5-η)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]ruthenium 177263-77-3, 2-(Diphenylphosphino)benzenemethanamine 350021-81-7, 2-(Diphenylphosphino)-N-methylethanamine
RL: **CAT (Catalyst use)**; USES (Uses)
(racemization of chiral sec-alcs. catalyzed by chloro[cyclooctadiene][pentamethylcyclopentadienyl]ruthenium/(diphenylphosphino)ethanamine in presence of potassium tert-butoxide)
REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L133 ANSWER 35 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:110336 CAPLUS Full-text

DOCUMENT NUMBER: 138:287562
TITLE: Asymmetric Synthesis of Highly Substituted β-Nitro Alcohols and Enantiomerically Enriched 4,4,5-Trisubstituted Oxazolidinones
AUTHOR(S): Crich, David; Ranganathan, Krishnakumar; Rumthao, Sochanchingwung; Shirai, Michio
CORPORATE SOURCE: Department of Chemistry, University of Illinois at Chicago, Chicago, IL, 60607-7061, USA
SOURCE: Journal of Organic Chemistry (2003), 68(5), 2034-2037
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:287562
ED Entered STN: 13 Feb 2003
GI



II

AB Asym. reduction of α,α-disubstituted-α-nitroketones R1COC(NO2)R2R3 [R1 = Me, Et, PhCH2CH2, cyclohexyl, 2-furyl, 2-thienyl, R2 = R3 = Me; R1 = PhCH2CH2, R2R3 = (CH2)4] with chiral oxazaborolidine, prepared in situ from BH3·Me2S and (S)-α,α-diphenyl-2- pyrrolidinemethanol gave the corresponding trisubstituted nitro alcs. R1CH(OH)C(NO2)R2R3 (I) in good to excellent yields (49-94%) and with high enantiomeric excess. Reduction of I with Raney nickel to the corresponding amino alcs. and subsequent reaction of the latter with phosgene under basic conditions afforded enantiomerically enriched 4,4,5-trisubstituted oxazolidinones II.
CC 28-6 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 23
ST ketone nitro **enantioselective** redn; alc nitro asym synthesis redn; oxazolidinone trisubstituted asym synthesis
IT **Alcohols, preparation**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(aliphatic, nitro; asym. synthesis of β-nitro **alcs**. and trisubstituted oxazolidinones via Henry reaction of aldehydes with nitroalkanes, oxidation of racemic β-nitro **alcs**., and **chiral** pyrrolidinemethanol-catalyzed reduction of β-nitro ketones)
IT **Asymmetric synthesis and induction**
(asym. synthesis of β-nitro **alcs**. and trisubstituted oxazolidinones via Henry reaction of aldehydes with nitroalkanes, oxidation of racemic β-nitro **alcs**., and **chiral** pyrrolidinemethanol-catalyzed reduction of β-nitro ketones)
IT **Ketones, preparation**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(nitro; asym. synthesis of β-nitro **alcs**. and trisubstituted oxazolidinones via Henry reaction of aldehydes with

nitroalkanes, oxidation of **racemic** β-nitro **alcs.**, and **chiral** pyrrolidinemethanol-catalyzed reduction of β-nitro ketones)

IT Reduction
Reduction catalysts
(stereoselective; asym. synthesis of β-nitro **alcs.** and trisubstituted oxazolidinones via Henry reaction of aldehydes with nitroalkanes, oxidation of racemic β-nitro **alcs.**, and **chiral** pyrrolidinemethanol-catalyzed reduction of β-nitro ketones)

IT 75-07-0, Acetaldehyde, reactions 79-46-9, 2-Nitropropane 98-01-1, 2-Furancarboxaldehyde, reactions 98-03-3, 2-Thiophenecarboxaldehyde 104-53-0, 3-Phenylpropanal 123-38-6, Propanal, reactions 2043-61-0, Cyclohexanecarboxaldehyde 2562-38-1, Nitrocyclopentane 20445-31-2, (R)-MTPA
RL: RCT (Reactant); RACT (Reactant or reagent)
(asym. synthesis of β-nitro **alcs.** and trisubstituted oxazolidinones via Henry reaction of aldehydes with nitroalkanes, oxidation of racemic β-nitro **alcs.**, and **chiral** pyrrolidinemethanol-catalyzed reduction of β-nitro ketones)

IT 13292-96-1P, 3-Methyl-3-nitro-2-butanone 20570-67-6P 20575-38-6P, 3-Methyl-3-nitro-2-butanol 32475-97-1P 82416-40-8P 85814-67-1P 89449-83-2P 101210-96-2P 504410-60-0P 504410-61-1P 504410-62-2P 504410-63-3P 504410-64-4P 504410-65-5P 504410-66-6P 504410-67-7P 504410-68-8P 504410-69-9P 504410-70-2P 504410-71-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(asym. synthesis of β-nitro **alcs.** and trisubstituted oxazolidinones via Henry reaction of aldehydes with nitroalkanes, oxidation of racemic β-nitro **alcs.**, and **chiral** pyrrolidinemethanol-catalyzed reduction of β-nitro ketones)

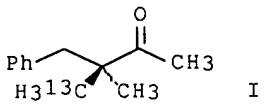
IT 154278-27-0P 159090-84-3P 504410-72-4P 504410-73-5P 504410-74-6P 504410-75-7P 504410-76-8P 504410-77-9P 504410-78-0P 504410-79-1P 504410-80-4P 504410-81-5P 504410-82-6P 504410-83-7P 504410-84-8P 504410-85-9P 504410-86-0P 504410-87-1P 504410-88-2P 504410-89-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(asym. synthesis of β-nitro **alcs.** and trisubstituted oxazolidinones via Henry reaction of aldehydes with nitroalkanes, oxidation of racemic β-nitro **alcs.**, and **chiral** pyrrolidinemethanol-catalyzed reduction of β-nitro ketones)

IT 112068-01-6, (S)-α,α-Diphenyl-2-pyrrolidinemethanol
RL: CAT (Catalyst use); USES (Uses)
(reduction catalyst; asym. synthesis of β-nitro **alcs.** and trisubstituted oxazolidinones via Henry reaction of aldehydes with nitroalkanes, oxidation of racemic β-nitro **alcs.**, and **chiral** pyrrolidinemethanol-catalyzed reduction of β-nitro ketones)

REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L133 ANSWER 36 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:525760 CAPLUS Full-text
DOCUMENT NUMBER: 137:216470
TITLE: Isotopically Chiral Probes for in Situ High-Throughput Asymmetric Reaction Analysis
AUTHOR(S): Evans, Michael A.; Morken, James P.
CORPORATE SOURCE: Department of Chemistry, Venable and Kenan

Laboratories, University of North Carolina at Chapel Hill, Chapel Hill, NC, 27599-3290, USA
SOURCE: Journal of the American Chemical Society (2002), 124(31), 9020-9021
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 137:216470
ED Entered STN: 16 Jul 2002
GI



I

AB A nonracemic 13C-labeled ketone I was prepared and used as a chiral probe in a high-throughput screening assay for ligands in ruthenium-catalyzed asym. transfer hydrogenation. I is nonracemic because of the presence of the isotopic label, but because the enantiomers differ very little in their steric environments, I exhibits chemical behavior similar to an **achiral** ketone in asym. reactions. The products of asym. reactions of I are diastereomers by virtue of the isotopic carbon labels. The carbon labels in products derived from asym. transformations of I are in diastereotopic environments and therefore lead to unique NMR resonances; the presence of a 13C isotopic label allows for rapid anal. of the diastereomers by 13C NMR. The effective "enantiomeric excess" of the reaction is determined through the use of single pulse, nonspinning, unlocked, and unshimmed 13C NMR spectroscopy; integration of the peaks for the diastereomers and calcn. of the ratio of diastereomers gives an estimate of the enantiomer excesses and conversions of the corresponding reaction with the analogous **achiral** ketone PHCH2CMe2COMe. Chiral GC anal. of reactions performed with I gave measurements of the diastereomeric excesses similar to those obtained using 13C NMR. The anal. of a single reaction by this technique can be performed in approx. 15 s. I was used as a chiral probe mol. in the asym. transfer hydrogenation of ketones in the presence of ruthenium arene complexes and amino alcs. Simple amino alcs. such as (R)- and (S)-phenylglycinol and a bis(η6- hexamethylbenzeneruthenium dichloride) precursor were found to generate the most effective catalysts in asym. transfer hydrogenation of I. The use of (R)- and (S)-phenylglycinol as catalysts for the asym. transfer hydrogenation reactions of acetophenone and 3-methyl-2-butanone with bis(η6-hexamethylbenzeneruthenium dichloride) with isopropanol and potassium hydroxide gave the corresponding secondary alcs. in 22-64% ee and in 92-98% conversions.

CC 21-2 (General Organic Chemistry)

ST carbon 13 labeled ketone prepn **chiral** probe asym reaction; high throughput screening carbon 13 labeled ketone **chiral** probe; screening ruthenium amino **alc** catalyst asym hydrogenation ketone

IT Alcohols, uses
RL: CAT (Catalyst use); USES (Uses)
(amino; high-throughput screening of ruthenium and amino **alc**. catalysts for asym. transfer hydrogenation of ketones using a nonracemic 13C-labeled ketone as a **chiral** probe in a 13C

NMR-based assay)
IT NMR (nuclear magnetic resonance)
(carbon-13; high-throughput screening of ruthenium and amino alc. catalysts for asym. transfer hydrogenation of ketones using a nonracemic 13C-labeled ketone as a chiral probe in a 13C NMR-based assay)
IT Asymmetric synthesis and induction
(preparation of a nonracemic 13C-labeled ketone as a chiral probe for use in
a 13C NMR-based method for the high-throughput screening of catalysts for asym. reactions)
IT Alcohols, preparation
RL: SPN (Synthetic preparation); PREP (Preparation)
(secondary; enantioselective preparation of secondary alcs. by asym. transfer hydrogenation of ketones in the presence of ruthenium complexes of amino alcs.)
IT Hydrogenation
Hydrogenation catalysts
(transfer, stereoselective; high-throughput screening of ruthenium and amino alc. catalysts for asym. transfer hydrogenation of ketones using a nonracemic 13C-labeled ketone as a chiral probe in a 13C NMR-based assay)
IT 90-82-4, (+)-Pseudoephedrine 147-85-3, L-Proline, uses 7531-52-4, (S)-Prolinamide 20989-17-7, (S)-Phenylglycinol 37366-09-9 51594-34-4 52462-29-0 56613-80-0, (R)-Phenylglycinol 67421-02-7 68832-13-3, (R)-Prolinol 71581-92-5 79815-20-6 163061-74-3, (1S,2S)-1-Amino-2-indanol
RL: CAT (Catalyst use); USES (Uses)
(high-throughput screening of ruthenium and amino alc. catalysts for asym. transfer hydrogenation of ketones using a nonracemic 13C-labeled ketone as a chiral probe in a 13C NMR-based assay)
IT 457064-02-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(high-throughput screening of ruthenium and amino alc. catalysts for asym. transfer hydrogenation of ketones using a nonracemic 13C-labeled ketone as a chiral probe in a 13C NMR-based assay)
REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L133 ANSWER 37 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:880431 CAPLUS Full-text
DOCUMENT NUMBER: 138:106546
TITLE: Chemoenzymatic Dynamic Kinetic Resolution of β-Halo Alcohols. An Efficient Route to Chiral Epoxides
AUTHOR(S): Pamies, Oscar; Baeckvall, Jan-E.
CORPORATE SOURCE: Department of Organic Chemistry, Arrhenius Laboratory, Stockholm University, Stockholm, SE-10691, Swed.
SOURCE: Journal of Organic Chemistry (2002), 67(25), 9006-9010
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:106546
ED Entered STN: 21 Nov 2002
AB Enzymic resolution of β-chloro alcs. in combination with ruthenium-catalyzed alc. isomerization led to a successful dynamic kinetic resolution (conversion up to 99% and ee up to 97%). The efficiency of the DKR is dramatically

reduced when β-bromo alcs. are used. The presence of the bromo substituent causes decomposition of the ruthenium catalysts, which triggers the progressive deactivation of the enzyme. The synthetic utility of this procedure has been illustrated by the practical synthesis of different chiral epoxides.

CC 27-2 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 23

IT **Resolution (separation)**
(enzymic, **kinetic**; chemoenzymic **dynamic kinetic** resolution of β-halo alcs. and subsequent conversion of intermediate acetates to chiral epoxides)

IT **Alcohols, preparation**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(halo, β-; chemoenzymic dynamic kinetic resolution of β-halo alcs. and subsequent conversion of intermediate acetates to chiral epoxides)

IT **Resolution (separation)**
(**kinetic, dynamic**; chemoenzymic **dynamic kinetic** resolution of β-halo alcs. and subsequent conversion of intermediate acetates to chiral epoxides)

IT **104439-77-2**
RL: **CAT (Catalyst use)**; USES (Uses)
(racemization catalyst; chemoenzymic dynamic kinetic resolution of β-halo alcs. and subsequent conversion of intermediate acetates to chiral epoxides)

REFERENCE COUNT: 43 THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L133 ANSWER 38 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:550664 CAPLUS Full-text
DOCUMENT NUMBER: 138:39057
TITLE: Fine-tuning of modular amino alcohol ligands for the enantioselective transfer hydrogenation of ketones
AUTHOR(S): Pasto, Mireia; Riera, Antoni; Pericas, Miquel A.
CORPORATE SOURCE: Unitat de Recerca en Sintesi Asimetrica (URSA-PCB), Departament de Quimica Organica / Parc Cientific de Barcelona, Universitat de Barcelona, Barcelona, 08028, Spain
SOURCE: European Journal of Organic Chemistry (2002), (14), 2337-2341
CODEN: EJOCFK; ISSN: 1434-193X
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:39057
ED Entered STN: 25 Jul 2002
AB A family of stereodefined, modular amino alcs. (3-alkoxy-1-amino-1-phenyl- 2-propanols), in which the steric bulk of the alkoxy and amino substituents varies smoothly, has been synthesized from enantiomerically pure phenylglycidol, prepared by Sharpless epoxidn. These amino alcs. have been evaluated as ligands in the catalyzed [(amino alc.)(arene)RuII] transfer hydrogenation of alkyl aryl ketones with 2-propanol as the hydrogen source. Both the nitrogen substituent and the alkoxy group have been optimized for maximal enantioselectivity and catalytic activity in the process under consideration.
CC 25-7 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
IT **Alcohols, preparation**
RL: CAT (Catalyst use); SPN (Synthetic preparation); **PREP**

(Preparation); USES (Uses)
(amino, aromatic; amino alc.-ruthenium complex catalysts for asym. transfer hydrogenation of acetophenone to (S)-α-methylbenzyl alc.)
IT 52462-29-0
RL: CAT (Catalyst use); USES (Uses)
(amino alc.-ruthenium complex catalysts for asym. transfer hydrogenation of acetophenone to (S)-α-methylbenzyl alc.)
REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L133 ANSWER 39 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:751983 CAPLUS Full-text
DOCUMENT NUMBER: 136:247366
TITLE: The first Ru(II)-catalysed asymmetric hydrogen transfer reduction of aromatic ketones in aqueous media
AUTHOR(S): Rhyoo, Hae Yoon; Park, Hee-Jung; Chung, Young Keun
CORPORATE SOURCE: School of Chemistry and Center for Molecular Catalysis, Seoul National University, Seoul, 151-747, S. Korea
SOURCE: Chemical Communications (Cambridge, United Kingdom) (2001), (20), 2064-2065
CODEN: CHCOFS; ISSN: 1359-7345
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 136:247366
ED Entered STN: 15 Oct 2001
AB The first water-soluble asym. H-transfer Ru(II) catalyst system consisting of [Ru(p-cymene)Cl2]2, (S)-proline amide, and HCOONa, which gives high conversion rates with high ee values up to 95.3% and is reusable, was developed.
CC 25-7 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
IT Alcohols, preparation
RL: SPN (Synthetic preparation); PREP (Preparation)
(aralkyl; enantioselective preparation by asym. hydrogen transfer reduction of aromatic ketones using (S)-proline amide and ruthenium(II) catalysts in aqueous media)
IT 52462-29-0 64030-43-9 84846-34-4 367521-34-4
RL: CAT (Catalyst use); USES (Uses)
(enantioselective preparation of aromatic alcs. by asym. hydrogen transfer reduction of aromatic ketones using (S)-proline amide and ruthenium(II) catalysts in aqueous media)
REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L133 ANSWER 40 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2000:471574 CAPLUS Full-text
DOCUMENT NUMBER: 133:237617
TITLE: A catalytic enantioselective allylation reaction of aldehydes in an aqueous medium
AUTHOR(S): Loh, T.-P.; Zhou, J.-R.
CORPORATE SOURCE: Department of Chemistry, National University of Singapore, Singapore, 117543, Singapore
SOURCE: Tetrahedron Letters (2000), 41(27), 5261-5264
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

OTHER SOURCE(S): CASREACT 133:237617
ED Entered STN: 13 Jul 2000
AB A modified Yamamoto-Yanagisawa's catalyst (S)-Tol-BINAP·AgNO3 was successfully applied to a catalytic enantioselective allylation reaction of aldehydes in an aqueous system. The reactions with aromatic aldehydes afforded the desired products in high yields with good stereoselectivities. E.g., (S)-Tol-BINAP·AgNO3 (0.1 mmol) was treated with 1-naphthaldehyde (1 mmol) and allyltributyltin (1 mmol) in the dark with stirring, affording the the corresponding allyl alc. in quant. yield and 81% ee.
CC 25-7 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
IT **Alcohols, preparation**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(allyl; enantioselective allylation reaction of aromatic aldehydes in aqueous
medium, catalyzed by modified Yamamoto-Yanagisawa's catalyst)
IT 2923-28-6, Silver triflate 7761-88-8, Silver nitrate, uses 7783-92-8, Silver chlorate 10102-05-3, Palladium dinitrate **20759-14-2**
21797-13-7 35658-65-2 42196-31-6 64443-05-6
RL: **CAT (Catalyst use)**; USES (Uses)
(in situ formation with chiral diphosphines of catalyst for enantioselective allylation reaction of aromatic aldehydes)
REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L133 ANSWER 41 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2000:756096 CAPLUS Full-text
DOCUMENT NUMBER: 134:43672
TITLE: Asymmetric activation/deactivation of racemic Ru catalysts for highly **enantioselective** hydrogenation of ketonic substrates
AUTHOR(S): Mikami, Koichi; Korenaga, Toshinobu; Ohkuma, Takeshi; Noyori, Ryoji
CORPORATE SOURCE: Dep. Chemical Technology, Tokyo Institute Technology, Tokyo, 152-8552, Japan
SOURCE: Angewandte Chemie, International Edition (2000), 39(20), 3707-3710
CODEN: ACIEF5; ISSN: 1433-7851
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 27 Oct 2000
AB An asym. activation/ deactivation strategy was developed for highly enantioselective hydrogenation irresp. of the ketonic substrates used by maximizing the difference in the catalytic activity between the enantiomeric catalysts. Thus, the present asym. activation/ deactivation protocol can be regarded as a paradigm shift in racemic catalysis.
CC 45-4 (Industrial Organic Chemicals, Leather, Fats, and Waxes)
Section cross-reference(s): 67, 75, 78
IT Bond angle
Bond length
Hydrogenation catalysts
(asym. activation/deactivation of racemic Ru catalysts for highly **enantioselective** hydrogenation of ketonic substrates)
IT **Ketones, reactions**
RL: RCT (Reactant); RACT (Reactant or reagent)
(asym. activation/deactivation of **racemic** Ru catalysts for highly **enantioselective** hydrogenation of ketonic substrates)
IT **Alcohols, preparation**
RL: IMF (Industrial manufacture); **PREP (Preparation)**
(asym.; asym. activation/deactivation of racemic Ru catalysts for

highly **enantioselective** hydrogenation of ketonic substrates)

IT Crystal structure
Molecular structure
(of asym. racemic Ru catalysts for highly **enantioselective** hydrogenation of ketonic substrates)

IT 78-59-1, Isophorone 93-08-3, Methyl 2-naphthyl ketone 98-86-2, Acetophenone, reactions 122-00-9 577-16-2 585-74-0 941-98-0, Methyl 1-naphthyl ketone
RL: RCT (Reactant); RACT (Reactant or reagent)
(asym. activation/deactivation of racemic Ru catalysts for highly **enantioselective** hydrogenation of ketonic substrates)

IT 29841-69-8, (S,S)-1,2-Diphenylethylenediamine 35132-20-8, (R,R)-1,2-Diphenylethylenediamine 312969-46-3
RL: CAT (Catalyst use); USES (Uses)
(catalyst activator; asym. activation/deactivation of racemic Ru catalysts for highly **enantioselective** hydrogenation of ketonic substrates)

IT 42177-25-3, (R)-1-(1-Naphthyl)ethanol
RL: CAT (Catalyst use); USES (Uses)
(catalyst; asym. activation/deactivation of racemic Ru catalysts for highly **enantioselective** hydrogenation of ketonic substrates)

IT 115245-70-0
RL: CAT (Catalyst use); RCT (Reactant); RACT (Reactant or reagent); USES (Uses)
(catalyst; asym. activation/deactivation of racemic Ru catalysts for highly **enantioselective** hydrogenation of ketonic substrates)

REFERENCE COUNT: 43 THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L133 ANSWER 42 OF 42 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1974:3672 CAPLUS Full-text
DOCUMENT NUMBER: 80:3672
TITLE: Optically active secondary alcohols
INVENTOR(S): Solodar, Arthur J.
PATENT ASSIGNEE(S): Monsanto Co.
SOURCE: Ger. Offen., 33 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2312924	A1	19730927	DE 1973-2312924	19730315
FR 2176128	A1	19731026	FR 1973-9394	19730315
JP 49001505	A	19740108	JP 1973-29547	19730315
GB 1423911	A	19760204	GB 1973-12510	19730315
CA 1000293	A1	19761123	CA 1973-166348	19730315
CH 593217	A5	19771130	CH 1973-3760	19730315
PRIORITY APPLN. INFO.:			US 1972-235405 A	19720316

ED Entered STN: 12 May 1984

AB Optically active secondary alcs., e.g. d- and l-menthol (I), ephedrine, pseudoephedrine, and threo- and erythro-AcNHCHMeCHPhOH, were prepared without any addnl. separation step by hydrogenation of the racemic ketones in the presence of coordination compds. of Rh with optically active phosphine ligands, e.g. bis(cyclohexyl-methyl-o-anisylphosphine)-1,5-cyclooctadienerhodium tetrafluoroborate (II). Thus, (±)-menthone was hydrogenated over optically active II in H2O-Me2CHCO2H 9.5 hr at 72° and 5.9

kg/cm2 to give menthol of optical purity 29.2% and which contained preponderantly I.

IC C07B; C07C; B01J

CC 30-10 (Terpenoids)
Section cross-reference(s): 63, 25, 34

IT **Ketones, reactions**
RL: RCT (Reactant); RACT (Reactant or reagent)
(hydrogenation of **racemic**, optically active alcs. by)

IT **Asymmetric synthesis and induction**
(of alcs., by hydrogenation of racemic ketones in presence of rhodium phosphine complexes)

IT **Alcohols, preparation**
RL: **PREP (Preparation)**
(optically active, by hydrogenation of racemic ketones)

FILE 'HOME' ENTERED AT 16:47:51 ON 02 FEB 2007

SEARCH HISTORY

```
=> d stat que l125
L14      152839 SEA FILE=REGISTRY ABB=ON  RU/ELS
L24           1 SEA FILE=REGISTRY ABB=ON  SUBTILISIN/CN
L25           1 SEA FILE=REGISTRY ABB=ON  PROTEINASE/CN
L67       72677 SEA FILE=CASREACT ABB=ON  STEREOSELECTIVE/NTE
L68       30236 SEA FILE=REGISTRY ABB=ON  L14 AND CASREACT/LC
L69        8227 SEA FILE=CASREACT ABB=ON  L68/CAT
L70         267 SEA FILE=CASREACT ABB=ON  L24/CAT OR L25/CAT
L73       76833 SEA FILE=CASREACT ABB=ON  (L69 OR L70 OR L67)
L76             STR
```


```
NODE ATTRIBUTES:
CONNECT IS E3  RC AT   2
CONNECT IS E1  RC AT   4
CONNECT IS E3  RC AT   6
DEFAULT MLEVEL IS ATOM
GGCAT   IS UNS  AT   1
GGCAT   IS UNS  AT   5
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS   8

STEREO ATTRIBUTES:
STEREO DEFAULT ABSOLUTE
NUMBER OF CHIRAL CENTERS IS 1
```

******MAPPINGS******

NOD	SYM	ROL	NOD	SYM	ROL
2	C	RRT	6	C	PRO
4	O	RRT	7	O	PRO
6	C	PRO	2	C	RRT
7	O	PRO	4	O	RRT

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L82             SCR 1149
L87          3195 SEA FILE=CASREACT SUB=L73 SSS FUL L76 AND L82 ( 20816 REACTIONS
                 )
L122            STR
```

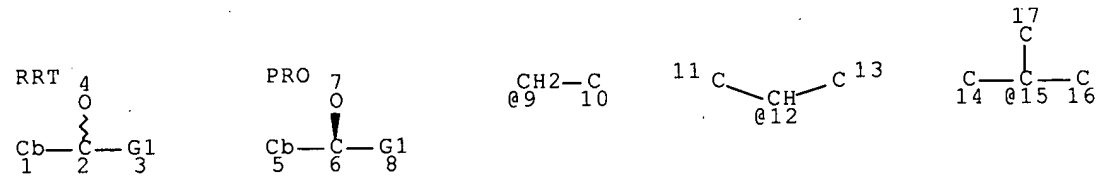


```
VAR G1=CH3/9/12/15
NODE ATTRIBUTES:
CONNECT IS E3  RC AT   2
CONNECT IS E1  RC AT   4
```

```
CONNECT IS E3  RC AT   6
DEFAULT MLEVEL IS ATOM
GGCAT   IS UNS  AT   1
GGCAT   IS UNS  AT   5
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  17

STEREO ATTRIBUTES:
STEREO DEFAULT ABSOLUTE
NUMBER OF CHIRAL CENTERS IS 1

  ****MAPPINGS****
NOD SYM      ROL    NOD SYM      ROL
  2 C        RRT      6 C        PRO
  4 O        RRT      7 O        PRO
  6 C        PRO      2 C        RRT
  7 O        PRO      4 O        RRT
L124       1785 SEA FILE=CASREACT SUB=L87 SSS FUL L122 ( 10785 REACTIONS)
L125       1783 SEA FILE=CASREACT ABB=ON  L124/COMPLETE


=> d his nofile

     (FILE 'HOME' ENTERED AT 09:49:53 ON 02 FEB 2007)

     FILE 'REGISTRY' ENTERED AT 09:50:16 ON 02 FEB 2007
               D SAVED
               ACT CHO829REG/A
              ---------
L1           59 SEA ABB=ON  (104439-77-2/BI OR 108-21-4/BI OR 108-82-7/BI OR
                108-88-3/BI OR 109-99-9/BI OR 117636-42-7/BI OR 1193-81-3/BI
                OR 123-91-1/BI OR 123-96-6/BI OR 13991-52-1/BI OR 1445-91-6/BI
                OR 1517-68-6/BI OR 151716-02-8/BI OR 1572-97-0/BI OR 161024-76-
                6/BI OR 16197-93-6/BI OR 219119-78-5/BI OR 219119-82-1/BI OR
                221911-67-7/BI OR 25501-32-0/BI OR 3113-98-2/BI OR 3319-15-1/BI
                 OR 3391-10-4/BI OR 371-27-7/BI OR 406-95-1/BI OR 470688-18-7/B
                I OR 52462-29-0/BI OR 529-34-0/BI OR 53732-47-1/BI OR 56-23-5/B
                I OR 5876-76-6/BI OR 600-36-2/BI OR 6169-06-8/BI OR 617713-61-8
                /BI OR 617713-62-9/BI OR 617713-63-0/BI OR 6351-10-6/BI OR
                6398-51-2/BI OR 64-18-6/BI OR 67-66-3/BI OR 698-87-3/BI OR
                701-70-2/BI OR 71-43-2/BI OR 7376-05-8/BI OR 7476-81-5/BI OR
                75-09-2/BI OR 835893-52-2/BI OR 835893-53-3/BI OR 835893-54-4/B
                I OR 835893-55-5/BI OR 835893-56-6/BI OR 837424-43-8/BI OR
                9001-73-4/BI OR 9001-92-7/BI OR 9004-07-3/BI OR 9014-01-1/BI
                OR 98-85-1/BI OR 99528-42-4/BI OR 99897-61-7/BI)
              ---------
               D SCAN

     FILE 'STNGUIDE' ENTERED AT 09:50:50 ON 02 FEB 2007

     FILE 'LREGISTRY' ENTERED AT 09:51:46 ON 02 FEB 2007
               E S/CN
               E (S)/CN
L2             1 SEA ABB=ON  "(S)-(+)-1-BUTEN-3-OL"/CN
               D IDE
L3               STR  6118-13-4
L4               STR
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L5            0 SEA SSS SAM L4
L6           15 SEA SSS FUL L4
                D SCAN
L7              STR L4
L8              STR L7
L9            0 SEA SSS SAM L8
L10          33 SEA SSS FUL L8
L11          18 SEA ABB=ON  L10 NOT L6
                D SCAN L6
                D SCAN
                D SET

     FILE 'CASREACT' ENTERED AT 12:25:45 ON 02 FEB 2007
L12             STR
L13          13 SEA SSS SAM L12 (   101 REACTIONS)

     FILE 'REGISTRY' ENTERED AT 12:29:16 ON 02 FEB 2007
L14      152839 SEA ABB=ON  RU/ELS

     FILE 'CAPLUS' ENTERED AT 12:29:24 ON 02 FEB 2007
L15      101120 SEA ABB=ON  L14
L16       25439 SEA ABB=ON  L15(L)CAT/RL
L17      150091 SEA ABB=ON  ALCOHOLS/CT
L18           0 SEA ABB=ON  L17(L)PREP/CT
L19       18354 SEA ABB=ON  L17(L)PREP/RL
L20         136 SEA ABB=ON  L19(L)"S"/OBI

     FILE 'STNGUIDE' ENTERED AT 12:33:39 ON 02 FEB 2007

     FILE 'CAPLUS' ENTERED AT 12:36:02 ON 02 FEB 2007
                E ASYMMETRIC SYNTHESIS AND INDUCTION+ALL/CT
L21       33996 SEA ABB=ON  "ASYMMETRIC SYNTHESIS AND INDUCTION"+OLD,NT/CT
                E RESOLUTION/CT
                E E11+ALL
L22       23387 SEA ABB=ON  "RESOLUTION (SEPARATION)"+OLD/CT
L23           6 SEA ABB=ON  L16 AND L20
                D SCAN TI
                SAVE TEMP L23 CHO829CA1/A

     FILE 'REGISTRY' ENTERED AT 12:39:28 ON 02 FEB 2007
L24           1 SEA ABB=ON  SUBTILISIN/CN
L25           1 SEA ABB=ON  PROTEINASE/CN

     FILE 'CAPLUS' ENTERED AT 12:39:38 ON 02 FEB 2007
L26       51371 SEA ABB=ON  (L24 OR L25)
L27        2353 SEA ABB=ON  L26(L)CAT/RL
L28         995 SEA ABB=ON  DYNAMIC/OBI(L)KINETIC/OBI
L29         226 SEA ABB=ON  L28(L)L22
L30           9 SEA ABB=ON  L29 AND (L16 OR L27) AND L19
                SAVE TEMP L30 CHO820CA2/A
                D QUE L23
L31           6 SEA ABB=ON  L20 AND (L16 OR L27)
                SAVE TEMP L31 CHO829CA1/A
L32         145 SEA ABB=ON  L19 AND L21 AND (L27 OR L16)
L33        1746 SEA ABB=ON  ACHIRAL/OBI
L34           4 SEA ABB=ON  L32 AND L33
                D SCAN
L35        3653 SEA ABB=ON  CHIRAL/OBI(L)(ALCOHOL/OBI OR ALCS/OBI)
                D QUE L32
L36          61 SEA ABB=ON  L19 AND L35 AND L21 AND (L27 OR L16)
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L37           2 SEA ABB=ON  L19 AND L35 AND L21 AND (L27 OR L16) AND L33
                SAVE TEMP L37 CHO829CA3/A
                D QUE L30
                D QUE L31
                D QUE L37
L38        5627 SEA ABB=ON  ACHIRAL/BI
L39           3 SEA ABB=ON  L19 AND L35 AND L21 AND (L27 OR L16) AND L38
L40           1 SEA ABB=ON  L39 NOT L37
                D SCAN
L41       19466 SEA ABB=ON  ENANTIOSELECT?/OBI
L42           4 SEA ABB=ON  L19(L)L41 AND L35 AND L21 AND (L27 OR L16)
                D  SCAN TI
                SAVE TEMP L39 CHO829CA3/A
                SAVE TEMP L42 CHO829CA4/A
L43       66509 SEA ABB=ON  KETONES/CT
L44       11738 SEA ABB=ON  RACEMIC/OBI
L45          10 SEA ABB=ON  L43(L)L44 AND L19 AND (L20 OR L21 OR L22 OR L35 OR
                L41)
                SAVE TEMP L45 CHO829CA5/A

     FILE 'CASREACT' ENTERED AT 12:52:19 ON 02 FEB 2007
                D QUE L12
L46          13 SEA SSS SAM L12 (   101 REACTIONS)
                D SCAN

     FILE 'LCASREACT' ENTERED AT 14:49:38 ON 02 FEB 2007
                E A/NTE
                E STER/NTE
                E A/NTE
L47           2 SEA ABB=ON  TUBE/NTE
                D IBIB ABS FHIT
                D IBIB ABS HIT
L48             STR L12
L49           3 SEA SSS SAM L48 (     8 REACTIONS)
                D IALL
                D HIT
                D HIT 2-3
                E STEREOSELECT?
L50          64 SEA ABB=ON  STEREOS?
                D HIT 1-10
                D IT 1-15
L51             STR L48
L52           0 SEA SSS SAM L51 (     0 REACTIONS)
L53           8 SEA SSS FUL L51 (    48 REACTIONS)
                D FHIT 1-8
L54          45 SEA ABB=ON  STEREOCHEMISTRY/CT
L55          14 SEA ABB=ON  ASYMMETRIC/CW
                D HIT
L56           3 SEA ABB=ON  L53 AND (L50 OR L54 OR L55)
                D HIT 1-3
L57             STR L51
L58           3 SEA SSS SAM L57 (     8 REACTIONS)
                D SCAN
                D FHIT 1-3

     FILE 'CASREACT' ENTERED AT 15:14:56 ON 02 FEB 2007
L59         335 SEA ABB=ON  KIM M?/AU
L60         448 SEA ABB=ON  PARK J?/AU
L61         212 SEA ABB=ON  CHUNG Y?/AU
L62         255 SEA ABB=ON  CHOI J?/AU
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L63          702 SEA ABB=ON  LEE H?/AU
L64          126 SEA ABB=ON  CHOI Y?/AU
L65          530 SEA ABB=ON  KIM D?/AU
L66            1 SEA ABB=ON  L59 AND L60 AND L61 AND L62 AND L63 AND L64 AND
                 L65
                 D SCAN
                 D IALL

     FILE 'STNGUIDE' ENTERED AT 15:16:21 ON 02 FEB 2007

     FILE 'CASREACT' ENTERED AT 15:18:38 ON 02 FEB 2007
                 E STER/NTE
L67        72677 SEA ABB=ON  STEREOSELECTIVE/NTE

     FILE 'REGISTRY' ENTERED AT 15:19:19 ON 02 FEB 2007
L68        30236 SEA ABB=ON  L14 AND CASREACT/LC

     FILE 'CASREACT' ENTERED AT 15:20:32 ON 02 FEB 2007

     FILE 'REGISTRY' ENTERED AT 15:21:01 ON 02 FEB 2007

     FILE 'CASREACT' ENTERED AT 15:21:57 ON 02 FEB 2007
L69         8227 SEA ABB=ON  L68/CAT
L70          267 SEA ABB=ON  L24/CAT OR L25/CAT
                 D QUE L57
L71              STR L57
L72           12 SEA SSS SAM L71 (    95 REACTIONS)
L73        76833 SEA ABB=ON  (L69 OR L70 OR L67)
L74           23 SEA SUB=L73 SSS SAM L71 (   169 REACTIONS)
L75         4126 SEA SUB=L73 SSS FUL L71 ( 43895 REACTIONS)
                 SAVE TEMP L75 CHO829CASRE/A

     FILE 'STNGUIDE' ENTERED AT 15:26:18 ON 02 FEB 2007

     FILE 'LREGISTRY' ENTERED AT 15:27:28 ON 02 FEB 2007

     FILE 'STNGUIDE' ENTERED AT 15:33:25 ON 02 FEB 2007

     FILE 'CASREACT' ENTERED AT 15:42:43 ON 02 FEB 2007
L76              STR L71
L77            7 SEA SSS SAM L76 (    71 REACTIONS)
L78           11 SEA SUB=L73 SSS SAM L76 (    94 REACTIONS)
L79              STR L76
L80            5 SEA SSS SAM L79 (    44 REACTIONS)
                 D SCAN
                 E ANY/CAT
L81           11 SEA SUB=L73 SSS SAM L76 (    94 REACTIONS)
L*** DEL         SCREEN 1701
L82              SCREEN 1149
                 D QUE L77
L83           11 SEA SUB=L73 SSS SAM L76 (    94 REACTIONS)
L84           24 SEA SSS SAM L76 AND L82 (   178 REACTIONS)
L85           13 SEA SUB=L73 SSS SAM L76 AND L82 (   112 REACTIONS)
                 D SCAN
L86           13 SEA SUB=L73 SSS SAM L76 AND L82 (   112 REACTIONS)
L87         3195 SEA SUB=L73 SSS FUL L76 AND L82 ( 20816 REACTIONS)
L88         3187 SEA ABB=ON  L87/COMPLETE
                 SAVE TEMP L88 CHO829CASRE/A
L89          520 SEA ABB=ON  L88 AND (L69 OR L70) AND L67
L90            5 SEA ABB=ON  L88 AND L69 AND L70 AND L67
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L91          517 SEA ABB=ON  (L59 OR L60 OR L61 OR L62 OR L63 OR L64 OR L65)
                 AND L67
L92           35 SEA ABB=ON  (L59 OR L60 OR L61 OR L62 OR L63 OR L64 OR L65)
                 AND L67 AND L88
L93           19 SEA ABB=ON  (L59 OR L60 OR L61 OR L62 OR L63 OR L64 OR L65)
                 AND L67 AND L88 AND (L69 OR L70)
L94          207 SEA ABB=ON  (L59 AND (L60 OR L61 OR L62 OR L63 OR L64 OR L65))
                 OR (L60 AND (L61 OR L62 OR L63 OR L64 OR L65)) OR (L61 AND
                 (L62 OR L63 OR L64 OR L65)) OR (L62 AND (L63 OR L64 OR L65))
                 OR (L63 AND (L64 OR L65)) OR (L64 AND L65)
L95           13 SEA ABB=ON  L94 AND L88 AND L67
L96           14 SEA ABB=ON  L94 AND L88 AND (L69 OR L70)
L97           13 SEA ABB=ON  L95 AND L96
L98            3 SEA ABB=ON  L90 AND L97
                 D QUE NOS L90
L99              STR L76
L100           0 SEA SUB=L87 SSS SAM L99 (     0 REACTIONS)
L101           0 SEA SUB=L87 SSS FUL L99 (     0 REACTIONS)
L102         512 SEA ABB=ON  L88 AND L69 AND L67
L103          13 SEA ABB=ON  L88 AND L70 AND L67
                 E ENZYM/CAT
                 E ENZYM/NTE
L104        9228 SEA ABB=ON  ENZYM?/NTE
L105          28 SEA ABB=ON  L102 AND L104

     FILE 'CAPLUS' ENTERED AT 16:03:45 ON 02 FEB 2007
L106       14460 SEA ABB=ON  KIM M?/AU
L107       25330 SEA ABB=ON  PARK J?/AU
L108        4144 SEA ABB=ON  CHUNG Y?/AU
L109       11169 SEA ABB=ON  CHOI J?/AU
L110       29440 SEA ABB=ON  LEE H?/AU
L111        8289 SEA ABB=ON  CHOI Y?/AU
L112       23463 SEA ABB=ON  KIM D?/AU
L113           1 SEA ABB=ON  L106 AND L107 AND L108 AND L109 AND L110 AND L111
                 AND L112

     FILE 'CASREACT' ENTERED AT 16:06:06 ON 02 FEB 2007
                 SAVE TEMP L97 CHO829CRAU/A
                 SAVE TEMP L103 CHO829CR1/A
                 SAVE TEMP L105 CHO829CR2/A

     FILE 'CAPLUS' ENTERED AT 16:06:39 ON 02 FEB 2007
L114         8708 SEA ABB=ON  (L106 AND (L107 OR L108 OR L109 OR L110 OR L111 OR
                 L112)) OR (L107 AND (L108 OR L109 OR L110 OR L111 OR L112)) OR
                 (L108 AND (L109 OR L110 OR L111 OR L112)) OR (L109 AND (L110
                 OR L111 OR L112)) OR (L110 AND (L111 OR L112)) OR (L111 AND
                 L112)
L115           22 SEA ABB=ON  L114 AND (L28 OR L35 OR L20)
L116           17 SEA ABB=ON  L114 AND (L29 OR L35 OR L20)
                 D SCAN TI

     FILE 'CAPLUS' ENTERED AT 16:09:57 ON 02 FEB 2007
                 D QUE L113
                 D QUE L116
L117           17 SEA ABB=ON  (L113 OR L116)

     FILE 'CASREACT' ENTERED AT 16:10:08 ON 02 FEB 2007
                 D QUE NOS L97

     FILE 'CASREACT, CAPLUS' ENTERED AT 16:10:19 ON 02 FEB 2007
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L118          24 DUP REM L97 L117 (6 DUPLICATES REMOVED)
                     ANSWERS '1-13' FROM FILE CASREACT
                     ANSWERS '14-24' FROM FILE CAPLUS
                 D IBIB ABS FHIT 1-13
                 D IBIB ED ABS HITIND 14-24

      FILE 'CASREACT' ENTERED AT 16:11:35 ON 02 FEB 2007
                 D STAT QUE L88
                 D QUE NOS L103
                 D QUE NOS L105
L119          28 SEA ABB=ON  (L103 OR L105) NOT L97

      FILE 'CAPLUS' ENTERED AT 16:12:13 ON 02 FEB 2007
                 D QUE L31
                 D QUE L30
                 D QUE L39
                 D QUE L42
                 D QUE L45
L120          27 SEA ABB=ON  (L31 OR L30 OR L39 OR L42 OR L45) NOT L117

      FILE 'CASREACT, CAPLUS' ENTERED AT 16:12:27 ON 02 FEB 2007
L121          52 DUP REM L119 L120 (3 DUPLICATES REMOVED)
                     ANSWERS '1-28' FROM FILE CASREACT
                     ANSWERS '29-52' FROM FILE CAPLUS
                 D IBIB ABS FHIT 1-28
                 D IBIB ED ABS HITIND 29-52

      FILE 'HOME' ENTERED AT 16:13:35 ON 02 FEB 2007
                 D STAT QUE L88
                 D SAVED

      FILE 'CASREACT' ENTERED AT 16:38:39 ON 02 FEB 2007
                 D QUE L99
                 D QUE L79
                 D QUE NOS L88
L122             STR L79
L123          50 SEA SUB=L87 SSS SAM L122 (   330 REACTIONS)
L124        1785 SEA SUB=L87 SSS FUL L122 ( 10785 REACTIONS)
L125        1783 SEA ABB=ON  L124/COMPLETE
                 SAVE TEMP L125 CHO829CRSUB/A
                 D QUE NOS L103
L126           5 SEA ABB=ON  L125(L)L69(L)L70
L127         363 SEA ABB=ON  L125(L)(L69 OR L70) AND L67
L128         350 SEA ABB=ON  L125(L)(L69 OR L70) (L) L67
                 D QUE NOS L105
L129           9 SEA ABB=ON  L125(L)L70
L130          21 SEA ABB=ON  L125(L)L69(L)L67(L)L104

      FILE 'CASREACT' ENTERED AT 16:45:47 ON 02 FEB 2007
                 D STAT QUE L125
                 D QUE NOS L129
                 D QUE NOS L130
L131          17 SEA ABB=ON  (L129 OR L130) NOT L97

      FILE 'CAPLUS' ENTERED AT 16:46:32 ON 02 FEB 2007
                 D QUE L31
                 D QUE L30
                 D QUE L39
                 D QUE L42
                 D QUE L45
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L132          27 SEA ABB=ON  (L31 OR L30 OR L39 OR L42 OR L45) NOT L117

     FILE 'CASREACT, CAPLUS' ENTERED AT 16:46:51 ON 02 FEB 2007
L133          42 DUP REM L131 L132 (2 DUPLICATES REMOVED)
                    ANSWERS '1-17' FROM FILE CASREACT
                    ANSWERS '18-42' FROM FILE CAPLUS
                D IBIB ABS FHIT
                D IBIB ABS FHIT 2-17
                D IBIB ED ABS HITIND 18-42

     FILE 'HOME' ENTERED AT 16:47:51 ON 02 FEB 2007
                D STAT QUE L125

=>
```